```
STEREO ATTRIBUTES: NONE
L5           76 SEA FILE=REGISTRY SSS FUL L3

100.0% PROCESSED    9677 ITERATIONS                          76 ANSWERS
SEARCH TIME: 00.00.01



     (FILE 'HOME' ENTERED AT 11:29:45 ON 21 MAR 2006)

     FILE 'REGISTRY' ENTERED AT 11:29:52 ON 21 MAR 2006
L1              STR
L2            6 SEA SSS SAM L1
                D SCAN
L3              STR L1
L4            4 SEA SSS SAM L3
L5           76 SEA SSS FUL L3
                SAVE TEMP L5 KWO769FULL/A

     FILE 'CAPLUS' ENTERED AT 11:38:01 ON 21 MAR 2006
L6           25 SEA ABB=ON  L5

     FILE 'REGISTRY' ENTERED AT 11:38:22 ON 21 MAR 2006
L7              ANALYZE L5 1-76 LC :       8 TERMS
                D

     FILE 'REGISTRY' ENTERED AT 11:39:33 ON 21 MAR 2006
                D STAT QUE L5

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:39:34 ON 21 MAR 2006
L8           33 SEA ABB=ON  L5
L9           26 DUP REM L8 (7 DUPLICATES REMOVED)
                     ANSWERS '1-25' FROM FILE CAPLUS
                     ANSWER '26' FROM FILE USPATFULL
                D IBIB ED ABS HITSTR 1-26

     FILE 'CAOLD' ENTERED AT 11:40:04 ON 21 MAR 2006
L10           8 SEA ABB=ON  L5
                D IALL HITSTR L10 1-8

     FILE 'HOME' ENTERED AT 11:40:19 ON 21 MAR 2006
                D SAVED
                D STAT QUE L5

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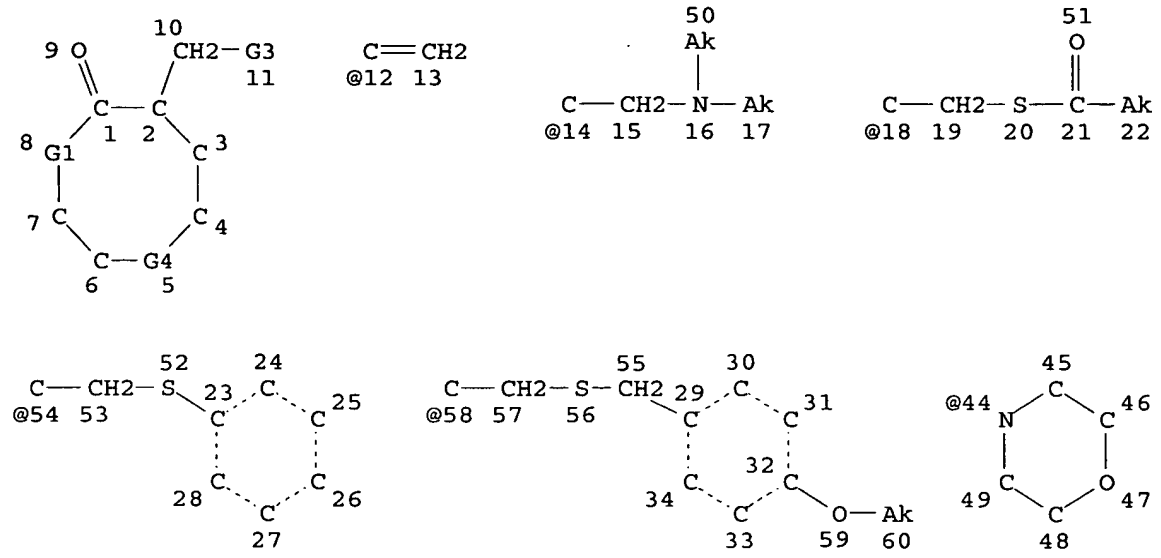
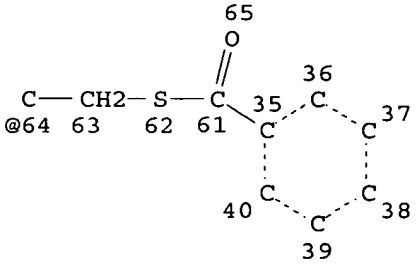
=> d stat que l5; d his nofile
L3 STR



Page 1-A



Page 2-A
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VAR G3=42/44
REP G4=(1-8) C
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CONNECT IS E1 RC AT 22
CONNECT IS E1 RC AT 41
CONNECT IS E1 RC AT 43
CONNECT IS E1 RC AT 50
CONNECT IS E1 RC AT 60
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 65

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=> fil reg; d stat que l5; fil capl uspatf toxcenter; s l5
FILE 'REGISTRY' ENTERED AT 11:39:33 ON 21 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   20 MAR 2006  HIGHEST RN 877371-73-8
DICTIONARY FILE UPDATES:  20 MAR 2006  HIGHEST RN 877371-73-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html


L3              STR
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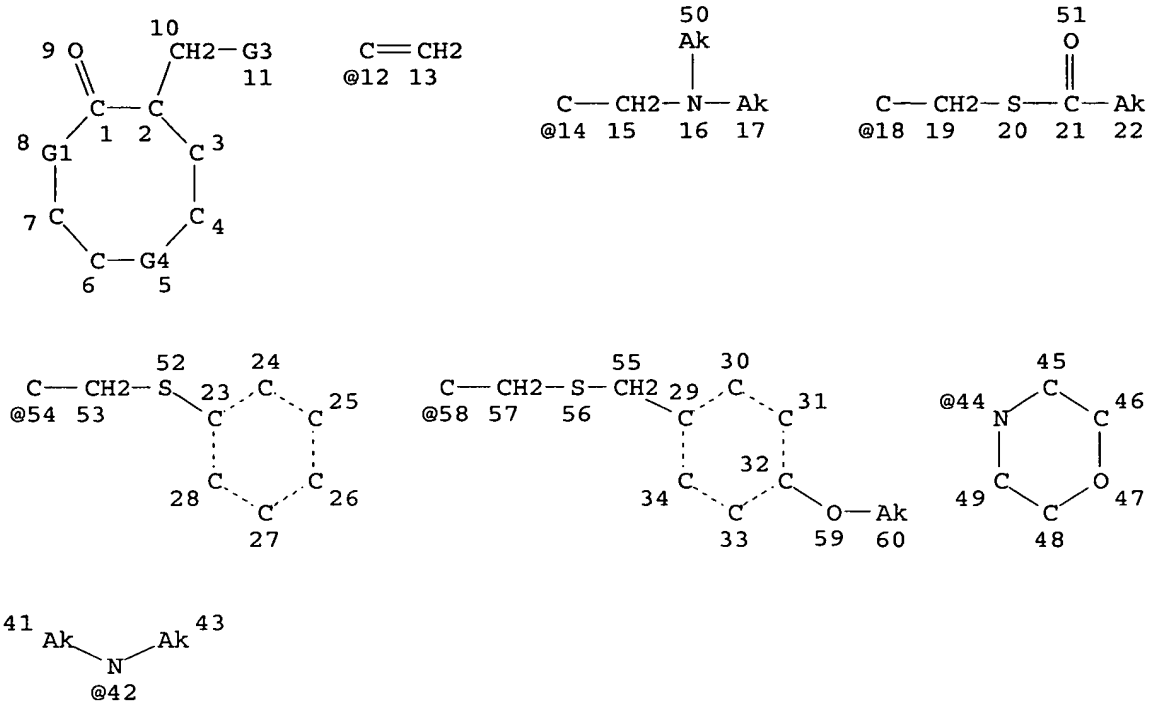
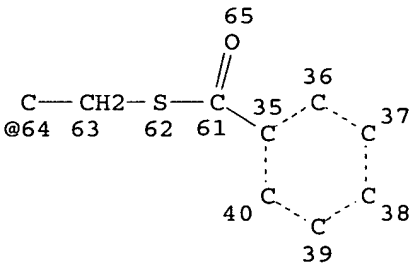


Page 1-A



Page 2-A
VAR G1=CH2/12/14/18/54/58/64
VAR G3=42/44
REP G4=(1-8) C
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 17
CONNECT IS E1 RC AT 22
CONNECT IS E1 RC AT 41
CONNECT IS E1 RC AT 43
CONNECT IS E1 RC AT 50
CONNECT IS E1 RC AT 60
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 65

STEREO ATTRIBUTES: NONE

L5 76 SEA FILE=REGISTRY SSS FUL L3

100.0% PROCESSED 9677 ITERATIONS 76 ANSWERS
SEARCH TIME: 00.00.01

FILE 'CAPLUS' ENTERED AT 11:39:34 ON 21 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE 'USPATFULL' ENTERED AT 11:39:34 ON 21 MAR 2006
CA INDEXING COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'TOXCENTER' ENTERED AT 11:39:34 ON 21 MAR 2006
COPYRIGHT (C) 2006 ACS

L8 33 L5

=> dup rem l8
PROCESSING COMPLETED FOR L8
L9 26 DUP REM L8 (7 DUPLICATES REMOVED)
ANSWERS '1-25' FROM FILE CAPLUS
ANSWER '26' FROM FILE USPATFULL

=> d ibib ed abs hitstr 1-26; fil cao; s l5

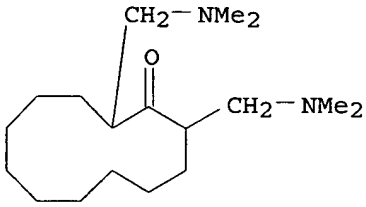
L9 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2005:1016720 CAPLUS
DOCUMENT NUMBER: 143:399241
TITLE: The Mannich Base NC1153 Promotes Long-Term Allograft Survival and Spares the Recipient from Multiple Toxicities
AUTHOR(S): Stepkowski, Stanislaw M.; Kao, Judy; Wang, Mou-Er; Tejpal, Neelam; Podder, Hemangshu; Furian, Lucrezia; Dimmock, Jonathan; Jha, Amitabh; Das, Umashankar; Kahan, Barry D.; Kirken, Robert A.
CORPORATE SOURCE: Division of Immunology and Organ Transplantation, Department of Surgery, University of Texas Medical School at Houston, Houston, TX, 77030, USA
SOURCE: Journal of Immunology (2005), 175(7), 4236-4246
CODEN: JOIMA3; ISSN: 0022-1767
PUBLISHER: American Association of Immunologists
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 21 Sep 2005
AB JAK3 is a cytoplasmic tyrosine kinase with limited tissue expression but is readily found in activated T cells. Patients lacking JAK3 are immune compromised, suggesting that JAK3 represents a therapeutic target for immunosuppression. Herein, we show that a Mannich base, NC1153, blocked IL-2-induced activation of JAK3 and its downstream substrates STAT5a/b more effectively than activation of the closely related prolactin-induced JAK2 or TNF-α-driven NF-κB. In addition, NC1153 failed to inhibit several other enzymes, including growth factor receptor tyrosine kinases, Src family members, and serine/threonine protein kinases. Although NC1153 inhibited proliferation of normal human T cells challenged with IL-2, IL-4, or IL-7, it did not block T cells void of JAK3. In vivo,

a 14-day oral therapy with NC1153 significantly extended survival of MHC/non-MHC mismatched rat kidney allografts, whereas a 90-day therapy induced transplantation tolerance (>200 days). Although NC1153 acted synergistically with cyclosporin A (CsA) to prolong allograft survival, it was not nephrotoxic, myelotoxic, or lipotoxic and did not increase CsA-induced nephrotoxicity. In contrast to CsA, NC1153 was not metabolized by cytochrome P 450 3A4. Thus, NC1153 prolongs allograft survival without several toxic effects associated with current immunosuppressive drugs.

IT **150661-91-9**, NC 1153
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Mannich base NC1153 promotes long-term allograft survival and spares the recipient from multiple toxicities)

RN 150661-91-9 CAPLUS

CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2004:513532 CAPLUS
DOCUMENT NUMBER: 141:65098
TITLE: Methods for selectively inhibiting Janus tyrosine kinase 3 (Jak3) with Mannich base compounds
INVENTOR(S): Kirken, Robert A.; Kahan, Barry D.; Stepkowski, Stanislaw M.; Priebe, Waldemar
PATENT ASSIGNEE(S): The Board of Regents of the University of Texas System, USA
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004052359	A1	20040624	WO 2003-US38993	20031209

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,

TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2506432	AA	20040624	CA 2003-2506432		20031209
AU 2003297740	A1	20040630	AU 2003-297740		20031209
US 2005203177	A1	20050915	US 2003-731769		20031209
EP 1578411	A1	20050928	EP 2003-796805		20031209
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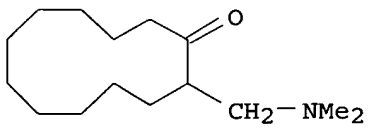
BR 2003017099	A	20051025	BR 2003-17099		20031209
NO 2005002497	A	20050902	NO 2005-2497		20050524
PRIORITY APPLN. INFO.:			US 2002-431851P	P	20021209
			WO 2003-US38993	W	20031209

OTHER SOURCE(S): MARPAT 141:65098
ED Entered STN: 25 Jun 2004
AB Methods are disclosed for inhibiting or disrupting Jak3 dependent function in cells of lymphoid or myeloid origin, especially for blocking proliferation and function of lymphocytes (e.g., T-cells, B-cells). A Mannich base compound, or a derivative or modified compound, is employed which is capable of selectively inhibiting Jak3 while affecting other protein tyrosine kinase activities to a lesser extent or not at all, to provide beneficial effects such as mitigation of transplant rejection and alleviation of allergic responses with fewer side effects than with conventional immunosuppressive agents. NCI drug, NC1153, selectively inhibited the proliferation and function of Jak3-containing T-cells, prolonged allograft survival, and demonstrated low toxicity.
IT **14519-21-2 150661-92-0 173543-81-2**
708984-86-5 708984-86-5D, salts **708984-87-6**
708984-87-6D, salts **708984-88-7 708984-89-8**
708984-90-1 708984-91-2 708984-92-3
708984-93-4 708984-94-5 708984-95-6
708984-98-9 708984-99-0 708985-00-6
708985-01-7 708985-02-8 708985-03-9
708985-04-0 708985-05-1 708985-06-2
708985-07-3
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(selectively inhibiting Janus tyrosine kinase 3 with Mannich base compds. for mitigation of transplant rejection and allergies)
RN 14519-21-2 CAPLUS
CN Cyclododecanone, 2-[(dimethylamino)methyl]-, hydrochloride (8CI, 9CI) (CA INDEX NAME)



● HCl

RN 150661-92-0 CAPLUS
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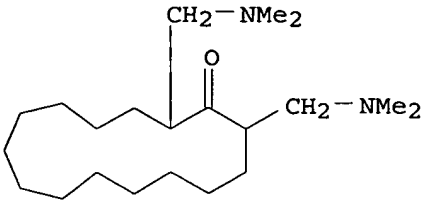

● 2 HCl

RN 173543-81-2 CAPLUS
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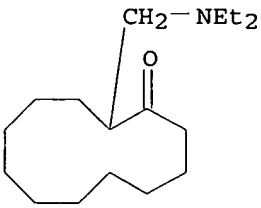

● HCl

RN 708984-86-5 CAPLUS
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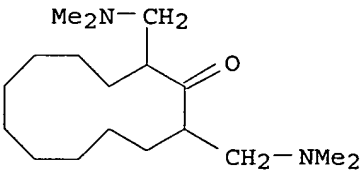

RN 708984-86-5 CAPLUS
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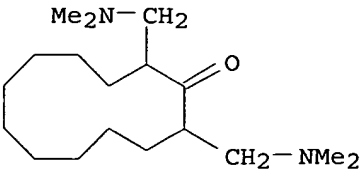
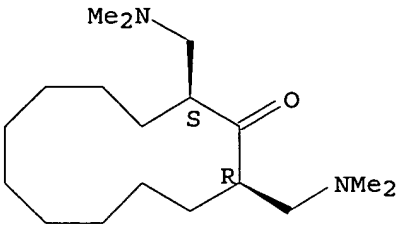


RN 708984-87-6 CAPLUS

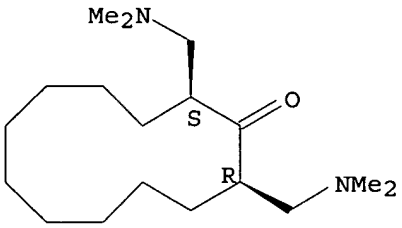
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, (2R,12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

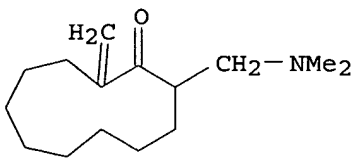


RN 708984-87-6 CAPLUS
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, (2R,12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

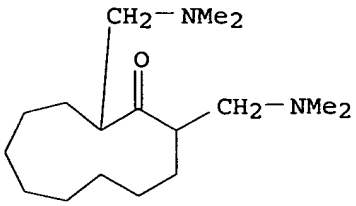


RN 708984-88-7 CAPLUS
CN Cycloundecanone, 2-[(dimethylamino)methyl]-11-methylene-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 708984-89-8 CAPLUS
CN Cycloundecanone, 2,11-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 708984-90-1 CAPLUS
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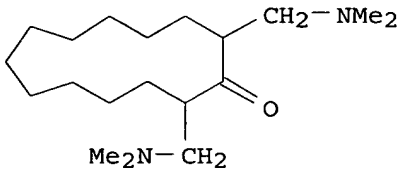
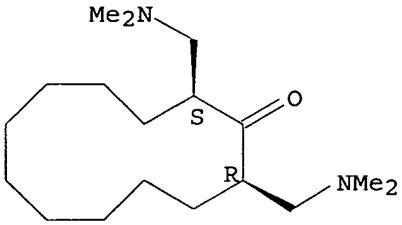


●2 HCl

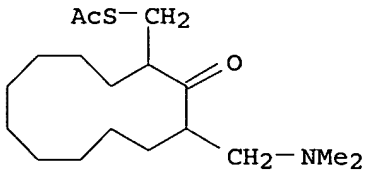
RN 708984-91-2 CAPLUS
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, dihydrochloride, (2R,12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



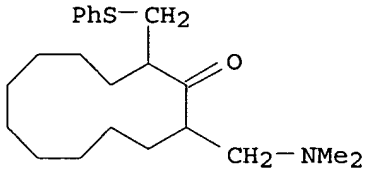
●2 HCl

RN 708984-92-3 CAPLUS
CN Ethanethioic acid, S-[[3-[(dimethylamino)methyl]-2-oxocyclododecyl]methyl] ester, hydrochloride (9CI) (CA INDEX NAME)



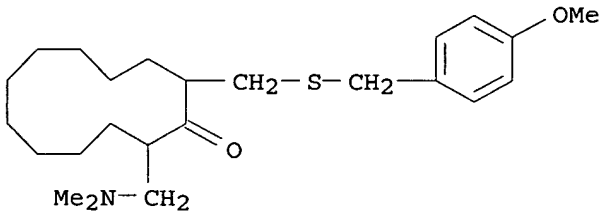
● HCl

RN 708984-93-4 CAPLUS
CN Cyclododecanone, 2-[(dimethylamino)methyl]-12-[(phenylthio)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



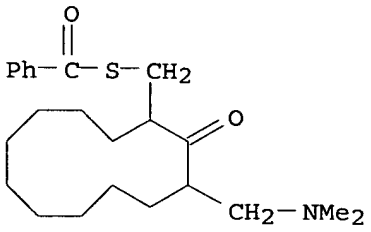
● HCl

RN 708984-94-5 CAPLUS
CN Cyclododecanone, 2-[(dimethylamino)methyl]-12-[[[(4-methoxyphenyl)methyl]thio]methyl]-, hydrochloride (9CI) (CA INDEX NAME)



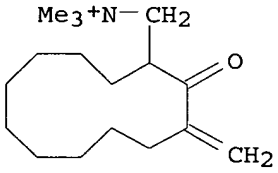
● HCl

RN 708984-95-6 CAPLUS
CN Benzenecarbothioic acid, S-[[3-[(dimethylamino)methyl]-2-oxocyclododecyl]methyl] ester, hydrochloride (9CI) (CA INDEX NAME)



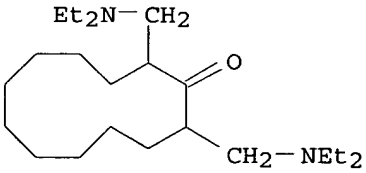
● HCl

RN 708984-98-9 CAPLUS
CN Cyclododecanemethanaminium, N,N,N-trimethyl-3-methylene-2-oxo-, iodide (9CI) (CA INDEX NAME)



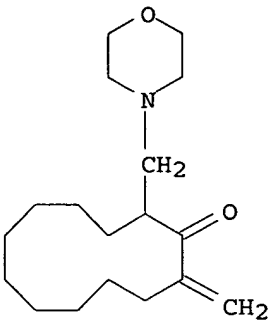
● I⁻

RN 708984-99-0 CAPLUS
CN Cyclododecanone, 2,12-bis[(diethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



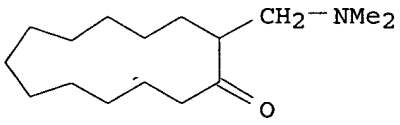
●2 HCl

RN 708985-00-6 CAPLUS
CN Cyclododecanone, 2-methylene-12-(4-morpholinylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)



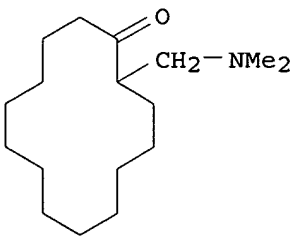
● HCl

RN 708985-01-7 CAPLUS
CN Cyclotridecanone, 2-[(dimethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



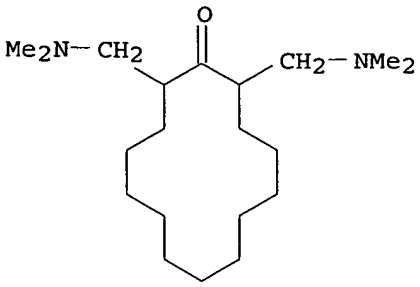
● HCl

RN 708985-02-8 CAPLUS
CN Cyclotetradecanone, 2-[(dimethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



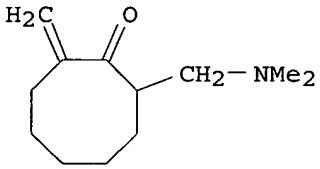
● HCl

RN 708985-03-9 CAPLUS
CN Cyclotetradecanone, 2,14-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



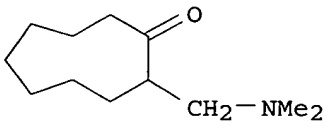
● 2 HCl

RN 708985-04-0 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]-8-methylene-, hydrochloride (9CI) (CA INDEX NAME)



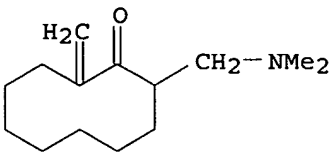
● HCl

RN 708985-05-1 CAPLUS
CN Cyclononanone, 2-[(dimethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



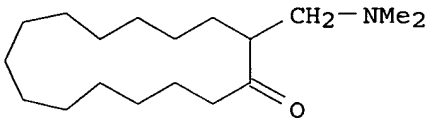
● HCl

RN 708985-06-2 CAPLUS
CN Cyclodecanone, 2-[(dimethylamino)methyl]-10-methylene-, hydrochloride (9CI) (CA INDEX NAME)



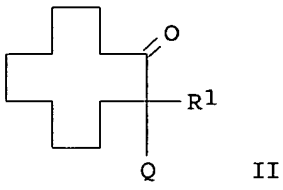
● HCl

RN 708985-07-3 CAPLUS
CN Cyclopentadecanone, 2-[(dimethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L9 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2002:242832 CAPLUS
DOCUMENT NUMBER: 137:46974
TITLE: Synthesis and biological activity of 2-arylaminomethyl-2-ethoxycarbonylfcyclododecanone
AUTHOR(S): Qi, Chuan-min; Zhang, Guan-xin; Wang, Yun-feng
CORPORATE SOURCE: Department of Chemistry, Beijing Normal University, Beijing, 100875, Peop. Rep. China
SOURCE: Yingyong Huaxue (2002), 19(3), 243-246
CODEN: YIHUED; ISSN: 1000-0518
PUBLISHER: Yingyong Huaxue Bianji Weiyuanhui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 137:46974
ED Entered STN: 02 Apr 2002
GI



II

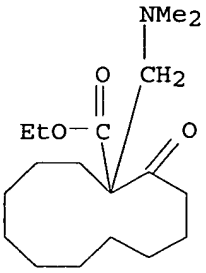
AB Eight title Mannich bases I (R = H, 4-Cl, 2-Cl, 4-CH3O, 2-Br, 4-Br, 4-CH3; R1 = COOCH2CH3; Q = CH2Q1; Q1 = NHC6H4R) were synthesized from reaction of

formaldehyde and dimethylamine hydrochloride and Q1H with I (Q = CH2N(CH3)2·HCl; R1 = COOCH2CH3), which was prepared from I (R1 = H; Q = H). Their structures were confirmed by IR, 1H NMR and elemental anal. Mannich reaction of an amine was occurred at ortho position of 2-ethoxycarbonyl-cyclododecanone. The preliminary in vitro bioassays of some compds. indicated that some of compds. IV showed certain fungistatic activity against plant pathogens. 4-Br substituted Ph aminomethyl-2-ethoxycarbonyl-cyclododecanone exerted appreciable inhibitory effect on xylene-induced ear edema in mice.

IT **438051-21-9P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. activity of arylaminomethylethoxycarbonylfcyclododecanone)

RN 438051-21-9 CAPLUS

CN Cyclododecanecarboxylic acid, 1-[(dimethylamino)methyl]-2-oxo-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L9 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 1995:962281 CAPLUS
DOCUMENT NUMBER: 124:145458
TITLE: Synthesis and cytotoxic evaluation of some Mannich bases of alicyclic ketones
AUTHOR(S): Dimmock, J. R.; Chamankhah, M.; Seniuk, A.; Allen, T. M.; Kao, G. Y.; Halleran, S.
CORPORATE SOURCE: Dep. Chem., Univ. Saskatchewan, SK, Can.
SOURCE: Pharmazie (1995), 50(10), 668-71
CODEN: PHARAT; ISSN: 0031-7144
PUBLISHER: Govi-Verlag Pharmazeutischer Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

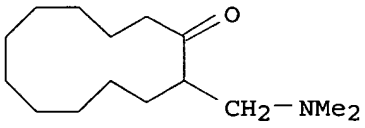
ED Entered STN: 05 Dec 1995

AB A number of Mannich bases of alicyclic ketones containing 1 and 2 basic centers were prepared to evaluate the theory of sequential cytotoxicity and develop structure-activity relationships in these series of compds. The compds. were evaluated in vitro against murine P388 D1 lymphocytic leukemia cells. The data generated supported the theory of sequential cytotoxicity and in general, compds. containing alicyclic rings of 5 and 6 C atoms possessed greater activity than the corresponding dodecyl analogs. Those Mannich bases containing dialkylamino groups were associated with greater cytotoxicity than related compds. possessing a basic heterocycle. Calcns. of the atomic charges of the enone groups from selected compds. afforded some

rationalization for the cytotoxic screening results.

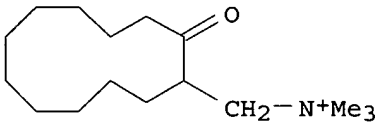
IT **14519-21-2 16277-21-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation and neoplasm inhibitory activity of Mannich bases of alicyclic ketones)

RN 14519-21-2 CAPLUS
CN Cyclododecanone, 2-[(dimethylamino)methyl]-, hydrochloride (8CI, 9CI) (CA INDEX NAME)



● HCl

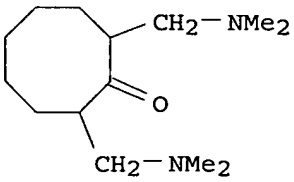
RN 16277-21-7 CAPLUS
CN Cyclododecanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



● I^-

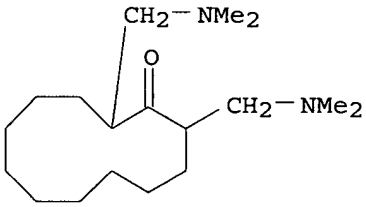
IT **6333-26-2P 150661-91-9P 173543-80-1P 173543-81-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and neoplasm inhibitory activity of Mannich bases of alicyclic ketones)

RN 6333-26-2 CAPLUS
CN Cyclooctanone, 2,8-bis[(dimethylamino)methyl]-, dihydrochloride (6CI, 8CI, 9CI) (CA INDEX NAME)



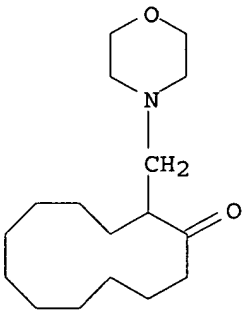
●2 HCl

RN 150661-91-9 CAPLUS
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



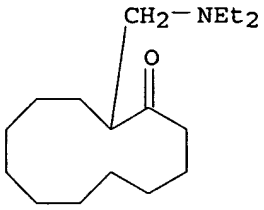
●2 HCl

RN 173543-80-1 CAPLUS
CN Cyclododecanone, 2-(4-morpholinylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)



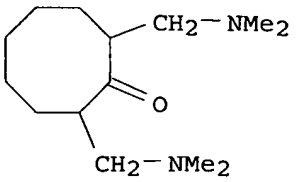
● HCl

RN 173543-81-2 CAPLUS
CN Cyclododecanone, 2-[(diethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



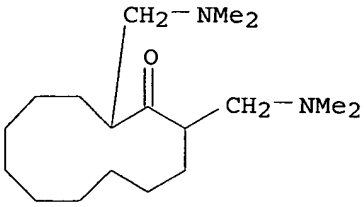
● HCl

L9 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 1993:603032 CAPLUS
DOCUMENT NUMBER: 119:203032
TITLE: Evaluation of some Mannich bases of cycloalkanones and related compounds for cytotoxic activity
AUTHOR(S): Dimmock, J. R.; Sidhu, K. K.; Chen, M.; Reid, R. S.; Allen, T. M.; Kao, G. Y.; Truitt, G. A.
CORPORATE SOURCE: Coll. Pharm., Univ. Saskatchewan, Saskatoon, SK, Can.
SOURCE: European Journal of Medicinal Chemistry (1993), 28(4), 313-22
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 13 Nov 1993
AB A number of Mannich bases of cycloalkanones and related quaternary ammonium compds. were prepared for cytotoxic evaluation in order to examine the theory that sequential release of alkylating agents produces increased bioactivity compared to related compds. containing only one potential alkylating site. Many of the compds. had significant activity against murine L1210 cells and various human tumors. Some correlations between structure and activity were noted, but the biol. data did not support the view that potential sequential liberation of cytotoxic species produced compds. with increased potency. The formation of various oximes and oxime benzoates as candidate prodrugs was achieved, but in general these compds. were not cytotoxic at the concns. utilized. This observation may be due to the fact that the oximes were much more stable in deuterated phosphate buffered saline over a period of 48 h at 37° than the Mannich bases, as revealed by 1H NMR spectroscopy.
IT **6333-26-2P 150661-91-9P 150661-92-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytotoxicity of)
RN 6333-26-2 CAPLUS
CN Cyclooctanone, 2,8-bis[(dimethylamino)methyl]-, dihydrochloride (6CI, 8CI, 9CI) (CA INDEX NAME)



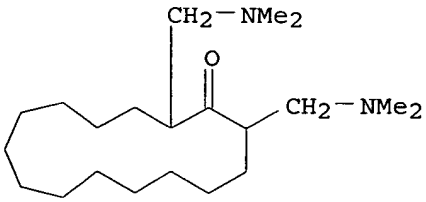
●2 HCl

RN 150661-91-9 CAPLUS
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

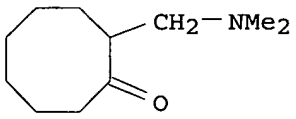
RN 150661-92-0 CAPLUS
CN Cyclopentadecanone, 2,15-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L9 ANSWER 6 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 1970:65748 CAPLUS
DOCUMENT NUMBER: 72:65748
TITLE: Action mechanism of antimicrobial β-amino ketones
AUTHOR(S): Schoenenberger, Helmut; Bastug, T.; Bindl, L.; Adam, Adelheid; Adam, Dieter; Petter, A.; Zwez, W.
CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ. Muenchen,

Munich, Fed. Rep. Ger.
SOURCE: Pharmaceutica Acta Helvetiae (1969), 44(11), 691-714
CODEN: PAHEAA; ISSN: 0031-6865
DOCUMENT TYPE: Journal
LANGUAGE: German
ED Entered STN: 12 May 1984
AB Structure-activity relations of aliphatic β-aminoketones, β-aminopropiophenones, α-phenyl-β-aminoketones, and α-phenyl-β-aminopropiophenones against fungis, yeasts, and gram-pos., and gram-neg. bacteria showed that the fungicidal activity was due to the β-amino ketone structure. Substitution of a Ph group on either the α-C or carbonyl C increased fungicidal activity, whereas substituents on either the amino group or the benzene ring had no effect. No correlations were found between the phys.-chem properties of these compds. and their resp. activity as fungicides. Addition of Cu2+ to the β-aminoketones did not alter their antimicrobial properties. The action of β-aminoketones as fungicides depended on formation of active breakdown products, H2CO and α,β-unsatd. ketones; a rapid rate of breakdown indicated increased fungicidal activity. 1-Dimethylamino-2-methyl-3-phenyl-3-propanone decreased the weight of Yoshida-sarcoma or sarcoma 180 by 40%; generally, β-aminoketones inhibited tumor growth of sarcoma 180 in mice by 50%; aliphatic β-aminoketones had no tumor inhibiting properties. The tumor inhibiting properties of aromatic β-aminoketones depended on the acetylation and aminomethylation of biol. cell substituents such as enzymes, DNA, or RNA.
IT **28118-62-9**
RL: BIOL (Biological study)
(biocides)
RN 28118-62-9 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]- (6CI, 8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 7 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 1967:499746 CAPLUS
DOCUMENT NUMBER: 67:99746
TITLE: 2-Oxocyclododec-1-ylacetic acid
PATENT ASSIGNEE(S): Chimie et Atomistique
SOURCE: Fr., 3 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

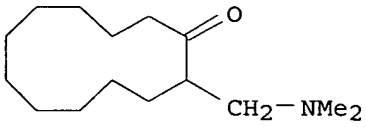
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1466205		19670120	FR 1960-823192	19600401

ED Entered STN: 12 May 1984
AB A mixture of cyclododecanone (18.2 g), 9 g MeN.HCl, 2.5 g trioxymethylene, and 50 mL EtOH was refluxed 1 hr. After addg. 2 g. trioxymethylene and 10 drops concentrated HCl the mixture was refluxed 1 hr. and kept at 0° to give 2-(dimethylaminomethyl)cyclododecan-1-one-HCl which was saponified with

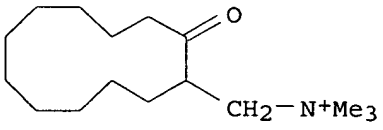
K2CO3 to give 14.5 g. free amine (I) m. 58°. I (22 g.) was dissolved in 50 mL AcOEt, 21 g MeI added, and heated on a water bath to give 33 g 2-dimethylaminomethylcyclododecan-1-one-MeI (II) m. 252°. A mixture of II (41 g), 170 mL H2O, 170 mL 95% EtOH, and 17 g NaCN was agitated and heated 1.5 h at 70° to give 21 g 2-(cyanomethyl)cyclododecan-1-one (III) m. 88°. A mixture of III (18 g), 25 g KOH, and 100 g H2O was refluxed 6 h to precipitate (2-oxocyclododec-1-yl)acetate which acidified with HCl to give 10 g title acid (IV) m. 129° (C6H6). IV and its salts have choleretic properties with a weak toxicity.

IT **16215-60-4P 16277-21-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and choleretic activity of)

RN 16215-60-4 CAPLUS
CN Cyclododecanone, 2-[(dimethylamino)methyl]- (7CI, 8CI, 9CI) (CA INDEX NAME)



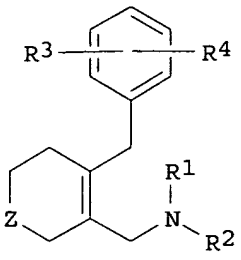
RN 16277-21-7 CAPLUS
CN Cyclododecanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



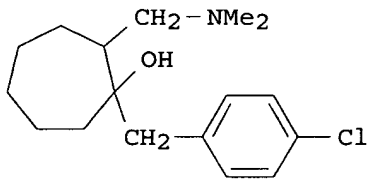
L9 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:76628 CAPLUS
DOCUMENT NUMBER: 144:170768
TITLE: Preparation of aralkylcyclohexanemethylamines as 5-HT/NA reuptake inhibitors
INVENTOR(S): Bloms-Funke, Petra; Friderichs, Elmar; Graudums, Ivars; Hennies, Hagen-Heinrich; Kless, Achim; Schiene, Klaus; Zimmer, Oswald
PATENT ASSIGNEE(S): Gruenenthal GmbH, Germany
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006008032	A1	20060126	WO 2005-EP7537	20050712
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102004034619	A1	20060223	DE 2004-102004034619	20040716
PRIORITY APPLN. INFO.:			DE 2004-102004034619A	20040716

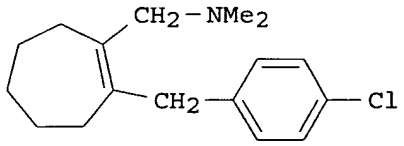
OTHER SOURCE(S): CASREACT 144:170768
ED Entered STN: 27 Jan 2006
GI



I



II

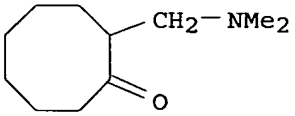


III

AB Title compds. I [R1 = alkyl; R2 = H, R1' R3, R4 = R2, halo, CF3, etc.] and their pharmaceutically salts were prepared For example, HBr mediated dehydration of amino alc. II afforded the hydrochloride salt of III in 30% yield after work-up. In 5-HT reuptake inhibition assays, 2-examples of compds. I exhibited Ki values ranging from 0.03-0.003 μM.

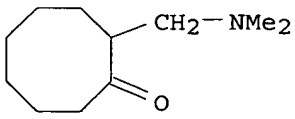
IT **28118-62-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aralkylcyclohexanemethylamines as 5-HT/NA reuptake inhibitors)

RN 28118-62-9 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]- (6CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

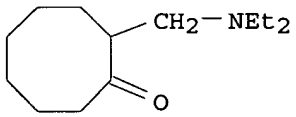
L9 ANSWER 9 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:435267 CAPLUS
DOCUMENT NUMBER: 121:35267
TITLE: Synthesis of substituted 2-aminonicotinonitriles
AUTHOR(S): Troschuetz, Reinhard; Dennstedt, Thomas
CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ. Erlangen-Nuernberg, Erlangen, D-91052, Germany
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1994), 327(1), 33-40
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
ED Entered STN: 23 Jul 1994
AB Mono-, di-, and trisubstituted 2-aminonicotinonitriles are prepared from ketonic Mannich-base hydrochlorides, enones, β-aminovinyl ketones, 3-aminoacroleins, or vinamidinium perchlorates, and 3,3-diaminoacrylonitrile (I), generated in situ. I is also reacted with ketonic Mannich-base hydrochlorides in the presence of ammonium acetate to yield the tetrahydro-1,8-naphthyridines.
IT **100049-46-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of aminonicotinonitriles)
RN 100049-46-5 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]-, hydrochloride (6CI, 9CI) (CA INDEX NAME)



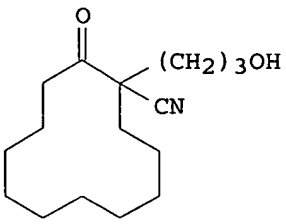
● HCl

L9 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:41597 CAPLUS
DOCUMENT NUMBER: 116:41597
TITLE: β-Trichlorostannyl ketones and aldehydes. Preparation and facile amine-induced dehydrostannation leading to α-methylene ketones and aldehydes
AUTHOR(S): Nakahira, Hiroyuki; Ryu, Ilhyong; Ikebe, Masanobu; Oku, Yoshiaki; Ogawa, Akiya; Kambe, Nobuaki; Sonoda, Noboru; Murai, Shinji
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Osaka, 565, Japan
SOURCE: Journal of Organic Chemistry (1992), 57(1), 17-28

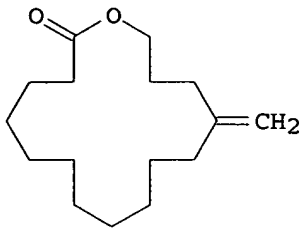
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:41597
ED Entered STN: 08 Feb 1992
AB Ring-opening reactions of siloxycyclopropanes with SnCl4 take place under mild reaction conditions and site-selectivity give β-trichlorostannyl ketones and aldehydes in high yields. The β-trichlorostannyl ketones and aldehydes thus obtained readily undergo base-induced dehydrotrichlorostannylation at room temperature to give the corresponding α-methylene ketones and aldehydes. The reactions are quite general for amines, such as pyridine, triethylamine, N,N,N',N'-tetramethylethylenediamine (TMEDA), and 1,4-diazabicyclo[2.2.2]octane (DABCO), and the yields are good to high. One-pot conversion from siloxycyclopropanes to α-methylene ketones or aldehydes by consecutive treatment with SnCl4 and TMEDA is also successful. The 1H NMR, 13C NMR, 119Sn NMR, and IR spectral properties of β-stannyl ketones and aldehydes are also reported.
IT **100539-22-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 100539-22-8 CAPLUS
CN Cyclooctanone, 2-[(diethylamino)methyl]- (6CI, 9CI) (CA INDEX NAME)



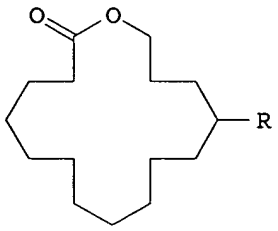
L9 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:55874 CAPLUS
DOCUMENT NUMBER: 108:55874
TITLE: Ring enlargement by fragmentation. Synthesis of 15-pentadecanolide (Exaltolide)
AUTHOR(S): Milenkov, Branimir; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org. Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1987), 70(3), 760-5
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 108:55874
ED Entered STN: 20 Feb 1988
GI



I



II



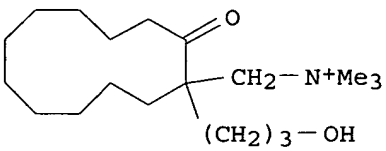
III

AB The title compound was prepared from 1-(3'-hydroxypropyl)-2-oxocyclododecane-1-carbonitrile (I), using 2 different routes. The cyano group of I was converted to the Me3N+CH2 group, which, upon NaH treatment, underwent a fragmentation leading to the ring-enlargement product II. The same product was observed after heating the ring-enlarged dimethylamine oxide III [R = CH2N(O)Me2], prepared from I via Bu4NF treatment and conversion of the CN into the dimethylamine-oxide moiety. Ozonolysis of the methylidene double bond in II and reduction of the resulting C:O to a CH2 group gave Exaltolide III (R = H).

IT **111887-56-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring enlargement reaction of)

RN 111887-56-0 CAPLUS

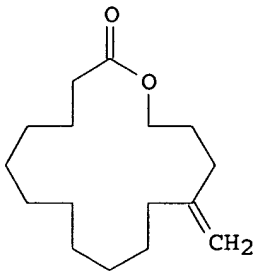
CN Cyclododecanemethanaminium, 1-(3-hydroxypropyl)-N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



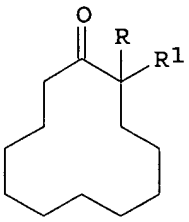
L9 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:21700 CAPLUS
DOCUMENT NUMBER: 108:21700
TITLE: Ring enlargement by fragmentation reaction. Transformation of 2-(aminomethyl)-2-(3-hydroxypropyl)cyclododecanone to 12-methylene-15-pentadecanolide

Searched by Barb O'Bryen, STIC 2-2518

AUTHOR(S): Milenkov, Branimir; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zuerich, Zurich, CH-8057, Switz.
SOURCE: Tetrahedron Letters (1987), 28(3), 315-18
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:21700
ED Entered STN: 23 Jan 1988
GI



I

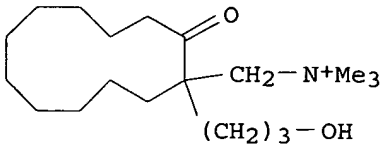


II

AB The title pentadecanolide I was prepared by treating cyclodecyltrimethylammonium iodide II [R = (CH2)3OH; R1 = CH2N+Me3I-] (III) with NaH. III was prepared in 3 steps from aldehyde II [R = (CH2)2CHO; R1 = CN] with NaBH4 reduction to give alc. II [R = (CH2)3OH; R1 = CN] as the first step. Further reduction with H-PtO2 gave II [R = (CH2)3OH; R1 = CH2NH2] which was alkylated with MeI to give III.

IT **111887-56-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring enlargement of, with sodium hydride)

RN 111887-56-0 CAPLUS
CN Cyclododecanemethanaminium, 1-(3-hydroxypropyl)-N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)

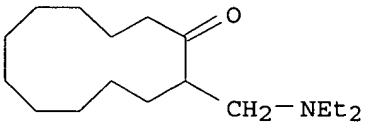


● I-

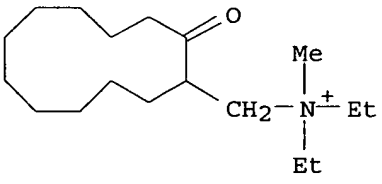
L9 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:454051 CAPLUS
DOCUMENT NUMBER: 103:54051
TITLE: Betweenanenes with vinylic heteroatoms. Route to sulfur analogs via [2,3]-sigmatropic rearrangement
AUTHOR(S): Nickon, Alex; Rodriguez, Abimael D.; Ganguly, Rathindra; Shirhatti, Vilas

Searched by Barb O'Bryen, STIC 2-2518

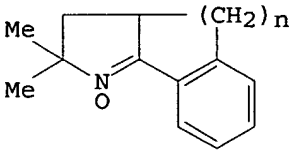
CORPORATE SOURCE: Dep. Chem., Johns Hopkins Univ., Baltimore, MD, 21218, USA
SOURCE: Journal of Organic Chemistry (1985), 50(15), 2767-77
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:54051
ED Entered STN: 24 Aug 1985
GI For diagram(s), see printed CA Issue.
AB The methylsulfonium salt of 7-methylene-1,5-dithiaspiro[5.11]heptadecane (I) was treated with different bases (Me3COK, BuLi, Me3CLi, DBU) to generate a transient sulfur ylide. In all cases the products were those from eliminations and from Stevens-type [1,2] rearrangements. In contrast, when dithioketal I was warmed with Et diazoacetate-CuSO4, the derived ylide produced the desired betweenanene II (R = Et, R1 = H) and its Z-isomer III in 4:1 ratio. Similarly, with di-Me diazomalonate and CuSO4, dithioketal I afforded the double-domed vinyl sulfide II (R = Me, R1 = CO2Me) along with its Z counterpart III in a 5:1 ratio. 2-Methyl-2-(1-methylvinyl)-1,3-dithiane also expanded its ring via the [2,3] manner when heated with Et diazoacetate or di-Me diazomalonate. The second sulfur in dithioketals does not thwart the [2,3]-sigmatropic rearrangement when ylides are generated with diazoesters. But, eliminations and Stevens-type [1,2] shifts prevailed when strong bases act on a preformed methylsulfonium salt.
IT **96575-34-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)
RN 96575-34-7 CAPLUS
CN Cyclododecanone, 2-[(diethylamino)methyl]- (9CI) (CA INDEX NAME)



IT **96555-22-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and elimination reaction of)
RN 96555-22-5 CAPLUS
CN Cyclododecanemethanaminium, N,N-diethyl-N-methyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



L9 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:174582 CAPLUS
DOCUMENT NUMBER: 100:174582
TITLE: Nitrones and oxaziridines. XXXI. Synthesis and some bicyclic 1-pyrroline 1-oxides
AUTHOR(S): Black, David St. C.; Johnstone, Lynn M.
CORPORATE SOURCE: Dep. Chem., Monash Univ., Clayton, 3168, Australia
SOURCE: Australian Journal of Chemistry (1984), 37(1), 117-28
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:174582
ED Entered STN: 26 May 1984
GI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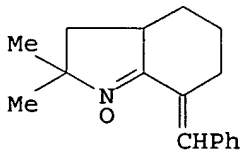
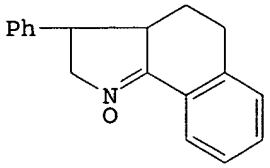
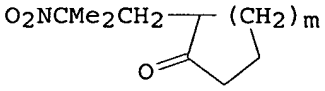
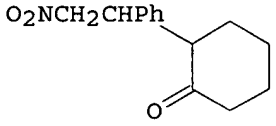
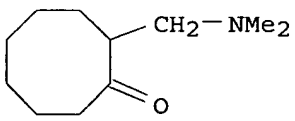

II


III


IV

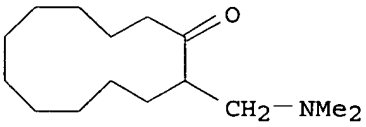

V

AB The bicyclic 1-pyrroline 1-oxides I-III (n = 1, 2) have been prepared by reductive cyclization of the resp. γ-nitro ketones. Reduction of IV (m = 1) gave an unstable nitrone, which underwent dimerization. IV (m = 2-4) and V were also prepared The pyrroline analog of III was also a product of the reduction of the nitro ketone.
IT **28118-62-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with nitropropane)
RN 28118-62-9 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]- (6CI, 8CI, 9CI) (CA INDEX NAME)

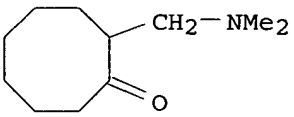


L9 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:508276 CAPLUS

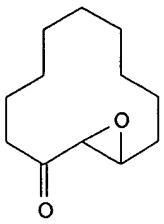
DOCUMENT NUMBER: 89:108276
TITLE: A convenient and general synthesis of 1,2-dimethylenecycloalkanes
AUTHOR(S): Van Straten, J. W.; Van Norden, J. J.; Van Schaik, T. A. M.; Franke, G. T.; De Wolf, W. H.; Bickelhaupt, F.
CORPORATE SOURCE: Scheikd. Lab., Vrije Univ., Amsterdam, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1978), 97(4), 105-6
CODEN: RTCPA3; ISSN: 0034-186X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 89:108276
ED Entered STN: 12 May 1984
AB Cycloalkanones were converted to the corresponding 1,2-dimethylenecycloalkanes (I) in 10-50% overall yield by Mannich condensation with HNMe2 and CH2O, Wittig reaction with Ph3P:CH2 and Hofmann degradation The conformations of I were discussed.
IT **16215-60-4P 28118-62-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of)
RN 16215-60-4 CAPLUS
CN Cyclododecanone, 2-[(dimethylamino)methyl]- (7CI, 8CI, 9CI) (CA INDEX NAME)



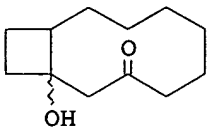
RN 28118-62-9 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]- (6CI, 8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1977:88773 CAPLUS
DOCUMENT NUMBER: 86:88773
TITLE: Photochemical rearrangement of trans-α,β-epoxycyclododecanone
AUTHOR(S): Marchesini, Alessandro; Pagnoni, Ugo M.
CORPORATE SOURCE: Cent. Stud. Sint. Stereochim. Spec. Sist. Org., CNR, Milan, Italy
SOURCE: Gazzetta Chimica Italiana (1976), 106(7-8), 663-70
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI



I



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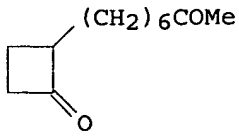

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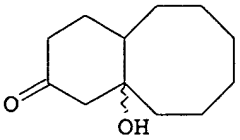


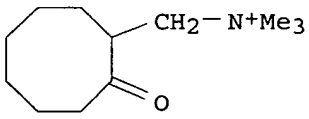
V

AB Photochem. Cα-O bond cleavage of the title compound I gave 1,3-cyclododecanedione (II). Type II photochem. reaction of II gave MeCOCH:C(OH)(CH2)6CH:CH2, III, and a stereoisomer of III. On irradiation, III gave cyclobutanone IV and the bicyclo[6.4.0]dodecane V. Biradical intermediates are proposed for all reactions.

IT **61977-58-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl acetoacetate in presence of sodium ethoxide)

RN 61977-58-0 CAPLUS

CN Cyclooctanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



● I⁻

L9 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1969:490904 CAPLUS
DOCUMENT NUMBER: 71:90904
TITLE: 2-Methylene C11-C13 cycloalkanones
AUTHOR(S): Muehlstaedt, Manfred; Remane, Horst; Graefe, Juergen
CORPORATE SOURCE: Karl-Marx-Univ., Leipzig, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Chemie (1969), 9(8), 303-5
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German

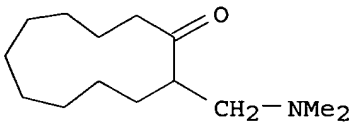
ED Entered STN: 12 May 1984

AB RR1CO [where (RR1 =) (CH2)10 to (CH2)12] (I) were subjected to a Mannich reaction with piperidine hydrochloride and H2CO to give RR1CO [where (RR1 =) (CH2)9CHCH2R2 to (CH2)11CHCH2R2] (II) (where R2 = 1-piperidinyl hydrochloride), which showed a measurable reduction step at pH 9 in polarographic reduction Thermolysis of II in high vacuum gave RR1CO [where

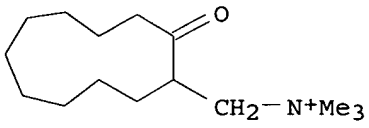
(RR1 =) (CH2)9C:CH2 to (CH2)11C:CH2] (III). III were obtained in better yields by converting I to II (R2 = NMe2.HCl), then to II (R2 = NMe2) and finelly to II (R2 = NMe2.MeI) and heating these with Na2CO3-aqueous MeOH. III were characterized as their NOCl adducts.

IT **24848-05-3P 24848-06-4P 24848-07-5P 24899-34-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

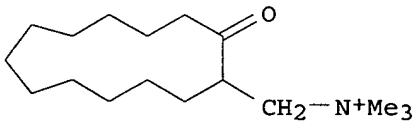
RN 24848-05-3 CAPLUS
CN Cycloundecanone, 2-[(dimethylamino)methyl]- (8CI) (CA INDEX NAME)



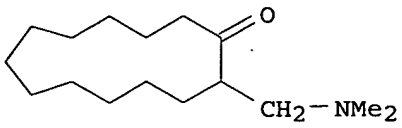
RN 24848-06-4 CAPLUS
CN Ammonium, trimethyl[(2-oxocycloundecyl)methyl]-, iodide (8CI) (CA INDEX NAME)



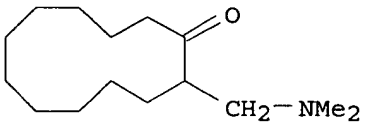
RN 24848-07-5 CAPLUS
CN Ammonium, trimethyl[(2-oxocyclotridecyl)methyl]-, iodide (8CI) (CA INDEX NAME)



RN 24899-34-1 CAPLUS
CN Cyclotridecanone, 2-[(dimethylamino)methyl]- (8CI) (CA INDEX NAME)



L9 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1967:10632 CAPLUS
DOCUMENT NUMBER: 66:10632
TITLE: Derivatives of cyclododecane
AUTHOR(S): Burger, Alfred; Paget, Charles J.
CORPORATE SOURCE: Univ. of Virginia, Charlottesville, VA, USA
SOURCE: Journal of Medicinal Chemistry (1966), 9, 968-70
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Many neuro- and psychopharmacol. active compds. contain cyclic moieties with acidic or basic functions in the rings or in side chains. Twenty-three cyclododecane derivs. with functional groups as they are encountered in typical drug mols., such as I, where R1 is H or NR (R is alkyl) and R2 is H, OH, etc., and II, were synthesized and biol. evaluated. None of them showed any interesting biol. activity.
IT **14519-21-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14519-21-2 CAPLUS
CN Cyclododecanone, 2-[(dimethylamino)methyl]-, hydrochloride (8CI, 9CI) (CA INDEX NAME)

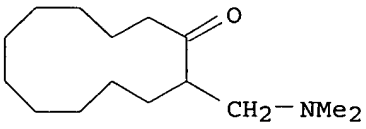


● HCl

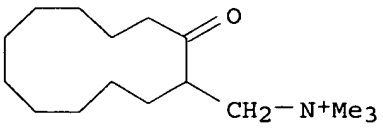
L9 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:59461 CAPLUS
DOCUMENT NUMBER: 58:59461
ORIGINAL REFERENCE NO.: 58:10104a-b
TITLE: 1-Oxocyclododecyl-2-acetic acid as a choleretic
PATENT ASSIGNEE(S): Chimie et Atomistique
SOURCE: 2 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

FR M100 19610227 FR 19600802
ED Entered STN: 22 Apr 2001
AB To synthesize the title compound (I), 18.2 g. cyclododecanone, 9 g. Me2NH.HCl, 2.5 g. trioxymethylene (II), and 50 cc. absolute EtOH were refluxed 1 hr., then treated with 2 g. II and 10 drops conductivity HCl, refluxed again 1 hr., the mixture cooled, and filtered. The precipitate was dissolved in 120 cc. H2O, alkalized with K2CO3, and filtered to give 14.5 g. 2-dimethylaminomethylcyclododecanone (III), m. 58°. III (22 g.) in 50 cc. AcOEt refluxed with 21 g. MeI, filtered, and crystallized gave III.MeI (33 g.), m. 252° (MeOH). III.MeI (41 g.), 170 cc. H2O, 170 cc. EtOH, and 17 g. NaCN was stirred 1.5 hrs. at 70°, cooled, and filtered to give 21 g. 2-cyanomethylcyclododecanone (IV), m. 88°. IV (18 g.), 25 g. KOH, and 100 cc. H2O refluxed 6 hrs., the mixture cooled and filtered, the filtrate acidified with HCl, the precipitate dissolved in H2O, and allowed to crystallize gave 10 g. I, m. 129° (C6H6). L.D.50 of I Na salt was orally or subcutaneously 625-1250 mg./kg. and intravenously 156-312 mg./kg.
IT **16215-60-4**, Cyclododecanone, 2-[(dimethylamino)methyl]-
16277-21-7, Ammonium, trimethyl[(2-oxocyclododecyl)methyl], iodide (preparation of)
RN 16215-60-4 CAPLUS
CN Cyclododecanone, 2-[(dimethylamino)methyl]- (7CI, 8CI, 9CI) (CA INDEX NAME)

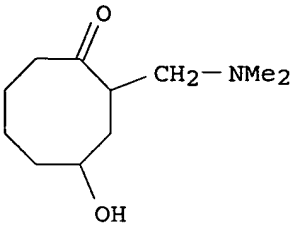


RN 16277-21-7 CAPLUS
CN Cyclododecanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



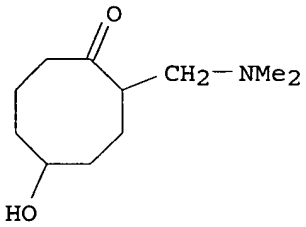
L9 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1962:53025 CAPLUS
DOCUMENT NUMBER: 56:53025
ORIGINAL REFERENCE NO.: 56:9992d-h
TITLE: Products of the catalytic oxidation of cyclooctane
AUTHOR(S): Moell, Hans; Urbanek, Friedrich
SOURCE: Festschrift Carl Wurster zum 60. Geburtstag (1960) 91-7

CODEN: 12VEAG
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB Oxidation of cyclooctane with O or air at normal pressure gives as main reaction products cyclooctanol (I) and cyclooctanone in 1:2 ratio. As side products are obtained aliphatic mono- and dicarboxylic acids and a total of 5% of the following compds.: cis-epoxy cyclooctane (II), b20 90°, m. 57°; 1,4-oxidocyclooctane (III), b20 70-2°, m. 31°; cyclooctanol-5-one (IV), b0.4 100-2°, m. 99-100°; cyclooctanol-4-one (V), b0.4 102-4°, m. 58-9°; bicyclo[0.3.3]oct-1(5)-en-2-one (VI), b8 102°, m. 18-19°. Addition of H2O to II gives 1,2-cyclooctanediol (VII) and 1,4-cyclooctanediol (VIII). Dehydration of VIII with KHSO4 gives III. Oxidation of bicyclo[0.2.4]octane with air yields IV and V. IV is soluble in H2O and forms a urethan, m. 103-4°, a phenylcarbamate, m. 108-9°, an oxime, m. 146-8°, and a phenylhydrazone, m. 100-2°. Oxidation of IV with HNO3 gives succinic acid, hydrogenation gives 1,5-cyclooctanediol, b0.5 106°, dehydration leads to 4-cycloocten-1-one, b11 83°, NH3 forms 1-amino-5-cyclooctanone, m. 40-2°, reaction with NH3 and H gives 1-amino-5-cyclooctanol, b0.4 140°, KCN and NH4HCO3 form 5-hydroxy-heptamethylenespirohydantoin, m. 273-5°, and HCHO plus NHMe2 gives 2-dimethylaminomethyl-5-hydroxy-cyclooctanone (HCl salt m. 182-3°), and dehydrogenation yields 1,4-oxido-5-cyclooctanol, b30 140°, m. 64°. Oxidation with air of VIII gives V, oxidation of VII leads to cyclooctanone. Reaction of V with C2H2 gives 1-ethynyl-1,4-dihydroxycyclooctane, b0.1 153-8°. The following derivs. of V were prepared: urethan, m. 117-19°; phenylcarbamate, m. 98-9°; oxime, m. 86-7°; phenylhydrazone, m. 90-1°; 1,4-cyclooctanediol, b0.5 110-15°; 1-amino-4-cyclooctanone, b1.5 65°; 1-amino-4-cyclooctanol, b0.1 136°; 4-hydroxy-heptamethylenespirohydantoin, m. 204-8°; 2-dimethyl aminomethyl-4-hydroxycyclooctanone HCl salt m. 127-31°. VI is formed during the oxidation of V or VIII. The following derivs. of VI are described: 2-aminobicyclo[0.3.3]octane, b1.5 53°; bicyclo[0.3.3]octan-2-ol, b0.2 62°; 2-chlorobicyclo[0.3.3]octane, b1 49°; bicyclo[0.3.3]oct-2-ene, b23, 52°; 1,4-bis(hydroxyamino)bicyclo [0.3.3] octane, m. 170-1°; 1,4-diaminobicyclo[0.3.3]octane, b0.2 52°.
IT **91370-52-4**, Cyclooctanone, 2-[(dimethylamino)methyl]-4-hydroxy-, hydrochloride **91370-53-5**, Cyclooctanone, 2-[(dimethylamino)methyl]-5-hydroxy-, hydrochloride
(preparation of)
RN 91370-52-4 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]-4-hydrOxy-, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 91370-53-5 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]-5-hydroxy-, hydrochloride (7CI) (CA INDEX NAME)



● HCl

L9 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1959:121615 CAPLUS
DOCUMENT NUMBER: 53:121615
ORIGINAL REFERENCE NO.: 53:21721a-c
TITLE: 1-Oxocyclooctyl-2-acetic acid
INVENTOR(S): Schlichting, Otto; Scheuerer, Gunter
PATENT ASSIGNEE(S): Badische Anilin- & Soda-Fabrik Akt.-Ges.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2882292		19590414	US	

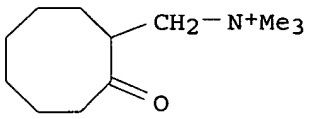
ED Entered STN: 22 Apr 2001
AB The title compound (I) was prepared by saponifying the corresponding nitrile which was prepared by treating NaCN (II) with quaternized Mannich reaction products derived from cyclooctanone. I demonstrated cholagogic action. The MeI salt 146 (m. 182-4°) of 2-(dimethylaminomethyl)cyclooctanone (III) (prepared from III 91 with MeI 106 in EtOAc) was heated 100 min. at 65-70° with II 66 in H2O 1320 parts. Me3N was evolved and 2-(cyanomethyl)cyclooctanone (IV) separated as an oil. Extraction and work-up of

the mixture yielded IV 68 parts, b0.3 106-7°; semicarbazone m. 127-8°. IV 68 with KOH 115 and H2O 460 was refluxed 7-8 hrs.; acidification (Congo red) and work-up yielded I 67 parts, m. 71-2° (cyclohexane); phenylhydrazone m. 109-10° (decomposition). Similarly, 2-(trimethylammoniummethyl)cyclooctanone-MeSO4 97 (m. 99°, prepared by reaction of III 73 with Me2SO4 252 in dry tetrahydrofuran with addition of small amts. of HOAc at 10-15°) was treated with II 48 in H2O 950 parts to yield IV; 2-(dimethylaminomethyl)cyclooctanone-HCl 44, m. 138-9° (decomposition), with II 30 in H2O 600 gave I 18 parts, and 2-(piperidinomethyl)cyclooctanone-MeI 108, m. 126-8°, with II 45 in H2O 900 gave I 30 parts.

IT **61977-58-0**, Ammonium, trimethyl(2-oxocyclooctylmethyl)-, iodide
100049-46-5, Cyclooctanone, 2-(dimethylaminomethyl)-, hydrochloride **108903-90-8**, Ammonium, trimethyl(2-oxocyclooctylmethyl)-, methyl sulfate
(preparation of)

RN 61977-58-0 CAPLUS

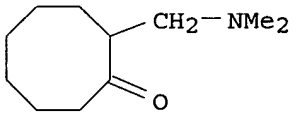
CN Cyclooctanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



● I^-

RN 100049-46-5 CAPLUS

CN Cyclooctanone, 2-[(dimethylamino)methyl]-, hydrochloride (6CI, 9CI) (CA INDEX NAME)



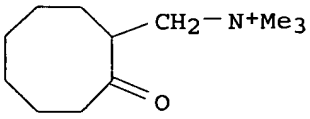
● HCl

RN 108903-90-8 CAPLUS

CN Trimethyl(2-oxocyclooctylmethyl)ammonium methyl sulfate (6CI) (CA INDEX NAME)

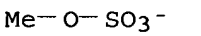
CM 1

CRN 108903-89-5
CMF C12 H24 N O



CM 2

CRN 21228-90-0
CMF C H3 O4 S



L9 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1960:28385 CAPLUS
DOCUMENT NUMBER: 54:28385
ORIGINAL REFERENCE NO.: 54:5507f-i,5508a-i,5509a-h
TITLE: Disubstitution of cycloalkanones in the Mannich reaction
AUTHOR(S): Blicke, F. F.; McCarty, F. J.
CORPORATE SOURCE: Univ. of Michigan, Ann Arbor
SOURCE: Journal of Organic Chemistry (1959), 24, 1069-76
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB Ten bis(aminomethyl)cycloalkanones were prepared by the simultaneous introduction of 2 aminomethyl groups into a cycloalkanone by the use of a Mannich reaction. It was definitely established that the reaction product obtained from cyclohexanone (I), paraformaldehyde (II), and Me2NH.HCl was 2,6-bis(dimethylaminomethyl)cyclohexanone (III).2HCl, and not the salt of the isomeric 2,2-disubstitution product. A mixture of 0.1 mole cycloalkanone, 0.2 mole amine-HCl, and 40 ml. AcOH was kept 2.5 hrs. at 95°, the mixture occasionally shaken, the solvent removed on a steam bath in vacuo, and the oily residue dissolved in 70 ml. hot Me2CO, the solution cooled, and the precipitated di-HCl salt recrystd. The following (CH2)n.CH2.CH(CH2NR2).CO.CH(CH2NR2).CH2.2HCl (IV.2HCl) were thus obtained (n, NR2, % yield, and m.p. given): 0, NMe2, 32, 187-8°; 1, NMe2, 63, 177-8°; 1, morpholino, 57, 163-4°; 1, NMeCH2Ph, 55, 169-70°; 2, NMe2, 42, 168-9°; 3, NMe2, 43, 179-80°. Since the crystalline IV.2HCl (n = 1, NR2 = piperidino) could not be purified by recrystn., it was converted into the solid base and purified by recrystn. from ligroine in 34% yield, m. 83-4°; dipicrate m. 162-3°. For the preparation of IV (n = 1, NR2 = NEt2) the reaction temperature was maintained at 75-80°, the solvent removed, the residue made alkaline, and the product distilled to give 9 g. 2(diethylaminomethyl)cyclohexanone, b0.4 73-0°; picrate m. 118-19° (H2O). The 2nd fraction (6 g.), b0.2 110-11°, was IV; since the di-HCl salt was very hygroscopic, a sample of IV was converted into the dipicrate, m. 137-8°. IV.2HCl (n = 1, NR2 = N(CH2Ph)2), 90% yield, m. 249-50°, was prepared by the general procedure but the temperature was kept at 55-60° and 160 ml. AcOH used as solvent; the free base m. 108-9°. The unfavorable effect of a higher temperature in the above preparation was shown as follows. The di-HCl salt (2

g.) and 10 ml. AcOH heated 2.5 hrs. at 95° gave 1.4 g. dibenzylamine-HCl, m. 257° (decomposition). Cyclopentanone (8.4 g.), 31.5 g. Me2NH.HBr, 9 g. II, and 50 ml. alc. refluxed 24 hrs. gave 31% IV.2HBr (n = 0, NR2 = NMe2), m. 198-9°. Similarly, the use of 0.25 mole morpholine-HCl and a reflux period of 17 hrs. gave 69% IV.2HCl (n = 0, NR2 = morpholino), m. 202-3° (MeOH). Where 0.1 mole I was used, the solvent removed in vacuo, and the oily residue triturated with iso-PrOH, and recrystd., 2.8 g. IV.2HBr (n = 1, NR2 = NMe2), 188-9°, was obtained. The marked difference in the yield of III. 2HCl obtained by the use of AcOH or alc. as a solvent was shown by the following expts. (a) I (98.1 g.), 60 g. II, 163.1 g. Me2NH.HCl, and 400 ml. AcOH heated 2.5 hrs. at 95°, the solvent removed, and the residue refluxed briefly with 500 ml. Me2CO gave 175 g. III.2HCl, m. 177-8°. Removal of the Me2CO from the filtrate, treatment of the residue with alkaline, and distillation gave 8.5 g. 2-(dimethylaminomethyl)cyclohexanone (V), b20 100-3°; HCl salt (Va), m. 155°. The above experiment was repeated but 400 ml. alc. was used to replace the AcOH, the solvent removed, and the residue treated with alkaline and distilled to give 23 g. V and 13.5 g. III, b0.4 93-7°. In an attempt to determine whether or not the yield of III could be increased by the use of larger amts. of II and Me2NH.HCl, more than 2 moles were used but only 8% III was obtained. To study the decomposition of III during its preparation by the general procedure, a solution of 28.5 g. III.2HCl in 40 ml. AcOH was heated 2.5 hrs. at 95°, the solvent removed, and the material refluxed with Me2CO to give a recovery of 27.8 g. III.2HCl. I (9.8 g.), 1.5 g. II, 11.7 g. dibenzylamine-HCl, and 50 ml. AcOH heated 2.5 hrs. at 55-65° gave 16.3 g. 2-(dibenzylaminomethyl)cyclohexanone-HCl (VI), m. 239-40°; picrate m. 159-60° (alc.). When VI was heated 2.5 hrs. at 95° in AcOH, it was decomposed almost completely to 90% dibenzylamine-HCl. I (15 g.), 12 g. methylbenzylamine-HCl, 2.3 g. II, and 30 ml. AcOH heated 2.5 hrs. at 75-80° gave 15 g. 2-(methylbenzylaminomethyl)cyclohexanone-HCl(VII),m.145-6° (Me2CO). IV.2HCl (n = 1, NR2 = NMeCH2Ph), 3 g. 5% Pd-C, and 150 ml. alc. hydrogenated 9 hrs. at 55 lb./sq. in. gave IV.2HCl (n = 1, NR2 = NHMe) in 42% yield, m. 167-8°. VII (7 g.), 3 g. 5% Pd-C, and 150 ml. alc. hydrogenated 15 min. at 50 lb./sq. in. gave 3.6 g. 2-(methylaminomethyl)-cyclohexanone-HCl (VIII), m. 100-1° (iso-PrOH-Et2O). VIII (1 g.) left 4 hrs. with 0.5 g. NH2OH.HCl, and 0.7 g. K2CO3 in 5 ml. H2O gave 0.4 g. VIII oxime, m. 192-3° (decomposition). I (19.6 g.), 3 g. II, 8.2 g. Me2NH.HCl, and 40 ml. AcOH heated 2.5 hrs. gave 14.5 g. Va. Va (99.2 g.), 3 g. I, 8.2 g. Me2NH.HCl, and 40 ml. AcOH gave 19.7 g. III.2HCl. Va (19.2 g.), 3 g. II, 12.2 g. piperidine-HCl, and 40 ml. AcOH gave 15.5 g. 2-(dimethylaminomethyl)-6-(piperidinomethyl)cyclohexanone-2HCl, m. 166-7° (MeOHEt2O). Mg (10 g.), 1 g. iodine, and 200 ml. MeOH refluxed 1 hr., and 70 g. dimethyl acetonedicarboxylate added, the mixture refluxed 1 hr., heated 24 hrs. in a pressure bottle with 80 g. (CH2)3Br2, the solvent removed, and the residue mixed with 125 ml. concentrated HCl, diluted with an equal volume of H2O, extracted with Et2O, the solvent removed, and the residue crystallized from MeOH-H2O gave 21.5 g. dimethyl cyclohexanone-2,6-dicarboxylate (IX), m. 142-3°. IX (13 g.), 0.3 g. PtO2, and 300 ml. MeOH hydrogenated 1 hr. at 50 lb./sq. in. gave 10.2 g. dimethyl cyclohexanol-2,6-dicarboxylate, m. 65-6° (ligroine). IX (16 g.), 12 g. Me2NH.HCl, 15 g. 37% HCHO, and 80 ml. MeOH refluxed 2 hrs. gave 26.8 g. dimethyl 2,6-bis(dimethylaminomethyl)cyclohexanone-2,6-dicarboxylate-2HCl (X), m. 186-7° (MeOHEtOAc). X (3.5 g.), 0.2 g. PtO2, and 50 ml. AcOH hydrogenated 5 hrs. at 60° under 56 lb./sq. in. gave 1.6 g. dimethyl 2,6-bis(dimethylaminomethyl)cyclohexanol-2,6-dicarboxylate-

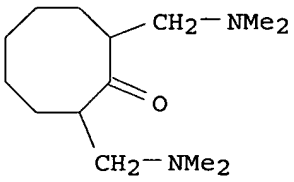
2HCl (Xa), m. 205-45° (MeOH-EtOAc). X (3 g.) and 27 ml. 5% aqueous NaOH stirred 7 hrs., concentrated HCl added, and the mixture made basic, extracted with Et2O, the solution treated with dry HCl, the Et2O decanted, and the oil triturated with 20 ml. iso-PrOH gave 54% III.2HCl. III.2HCl gave an oxime, m. 221-2° (decomposition). III.2HCl (20 g.), 30 ml. C5H5N, and 200 ml. alc. refluxed 4 hrs., the solvents removed, the residue dissolved in H2O, the solution made basic, extracted with Et2O, and treated with dry HCl gave 14 g. of the oxime-HCl. III.2HCl (25 g.), 225 ml. MeOH, and 0.25 g. PtO2 hydrogenated during 4 hrs. gave 19 g. 2,6-bis(dimethylaminomethyl)cyclohexanol-2HCl (XI), m. 231-2° (decomposition); dipicrate m. 197-8° (H2O). XI base (5 g.), 40 ml. MeCOEt, and 4 g. diphenylacetyl chloride heated 15 min. gave 3.5 g. solid and treatment of the filtrate with dry HCl gave an addnl. 3 g. solid; recrystn. gave 3.8 g. XI diphenylacetate, m. 246-7° (decomposition). The base from 4.4 g. XI in 60 ml. MeCOEt added during 1 hr. to 5.5 g. diphenylchloroacetyl chloride in 60 ml. MeCOEt gave 1.3 g. diphenylchloroacetate of XI, m. 241-2° (decomposition) (MeOH-Et2O). The base from 10 g. XI added dropwise to 9.3 g. molten diphenylchloroacetyl chloride and heated 10 min. on the steam bath, 25 ml. H2O added, and the mixture acidified, extracted with Et2O, the Et2O solution acidified, the aqueous solution made alkaline, extracted, and the dried extract treated with dry HCl gave 7 g. benzilate of XI, m. 254° (decomposition) (MeOH-Et2O). A sample of the base of XI converted into the benzilate was similarly treated. III (42.4 g.) added dropwise to PhMgBr (from 63 g. PhBr), the mixture refluxed 2 hrs., decomposed with NH4Cl solution, and the Et2O layer separated gave 21.5 g. 2,6-bis(dimethylaminomethyl)-1-phenylcyclohexanol (XII), b0.1 136-8°; di-HCl salt, m. 269-70° (decomposition); dipicrate m. 195-6° (alc.). PhLi (from 47 g. PhBr, 4.2 g. Li, and 500 ml. Et2O cooled to -5°) treated with 59.3 g. III in 100 ml. Et2O, the mixture stirred 1 hr., decomposed, and separated as above gave 45 g. XII, m. 71-3°; dimethiodide m. 283-4° (decomposition). XII.2HCl (8 g.) and 80 ml. (EtCO)2O heated 6 hrs. at 110-20° gave 8.1 g. 2,6-bis(dimethylaminomethyl)-1-phenyl-1-propionyloxycyclohexane-2HCl, m. 228-9° (iso-PrOH-EtOAc); dimethobromide m. 220-1° (decomposition). BuLi (from 2.8 g. Li, 27.5 g. BuBr, and 400 ml. Et2O) treated during 10 min. at 60° with 28.5 g. 2-bromopyridine, 34 g. III added during 15 min., the mixture stirred 2 hrs. at -40°, decomposed at room temperature with dilute NH4Cl, and the Et2O separated, and evaporated gave 19 g. 2,6-bis(dimethylaminomethyl)-1-(2-pyridyl)cyclohexanol, m. 66-7° (ligroine); tri-HCl salt (XIII), m. 258-9° (decomposition) (MeOH-EtOAc). XIII (10 g.) and 100 ml. (EtCO)2O heated 12 hrs. at 110-20° gave 7.6 g. 2,6-bis(dimethylaminomethyl)-1-(2-pyridyl)-1-propionyloxycyclohexane-2HCl, m. 249-50° (decomposition). The base of the oxime, obtained from 12 g. of the oxime of III in 125 ml. Et2O, added dropwise to 6.1 g. LiAlH4 in 200 ml. Et2O, the mixture refluxed 4 hrs., stirred 9 hrs. at room temperature, and decomposed with H2O, and then 6 ml. 15% NaOH gave 10.5 g. crude 2,6-bis(dimethylaminomethyl)-1-aminocyclohexane, converted into the tripicrate, m. 230-1° (decomposition). IV.2HCl (n = 0, NR2 = NMe2) (5 g.) in 8 ml. H2O added dropwise during 20 min. to 1.6 g. NaBH4 in 8 ml. H2O, stirred 2 hrs., decomposed, and the dried Et2O solution treated with dry HCl gave 4 g. 2,5-bis(dimethylaminomethyl)cyclopentanol-2HCl, m. 226-8° (alc.). X (15 g.), 0.2 g. PtO2, and 150 ml. MeOH hydrogenated 1 hr. at 50 lb./sq. in., filtered, about half the solvent removed, Et2O added, the mixture refrigerated 7 days and the solid recrystd. gave 1.8 g. Xa. The filtrate concentrated to a small volume gave 0.7 g. dimethyl cyclohexanone-2,6-dicarboxylate (XIV), m. 142-3°. The filtrate

treated with Et2O gave 1.5 g. Me3N.HCl, m. 274-5° (decomposition). An aqueous solution of the Me3N.HCl with picric acid gave the picrate, m. 217-19°. X (4 g.) in 25 ml. H2O heated 3.5 hrs. with passage of air through the solution and 1 g. XIV collected and the filtrate yielded Me2NH.HCl, m. 167-8°. The precipitated 2,4-dinitrophenylhydrazone of HCHO (0.2 g.) m. 163-5° (alc.).

IT **6333-26-2**, Cyclooctanone, 2,8-bis(dimethylaminomethyl)-, dihydrochloride
(preparation of)

RN 6333-26-2 CAPLUS

CN Cyclooctanone, 2,8-bis[(dimethylamino)methyl]-, dihydrochloride (6CI, 8CI, 9CI) (CA INDEX NAME)



●2 HCl

L9 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1959:40053 CAPLUS

DOCUMENT NUMBER: 53:40053

ORIGINAL REFERENCE NO.: 53:7217c-e

TITLE: 2-(Disubstituted-aminomethyl)cyclooctanones

INVENTOR(S): Schlichting, Otto; Scheuerer, Guenter; Westphal, Franz; Amann, August

PATENT ASSIGNEE(S): Badische Anilin- & Soda-Fabrik Akt.-Ges.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2861993		19581125	US	

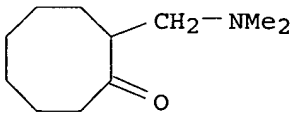
ED Entered STN: 22 Apr 2001

AB The title compds., having analgesic properties, were prepared Cyclooctanone (I) 252 refluxed 105 min. with Me2NH.HCl 81.5, paraformaldehyde 39, and absolute EtOH 320 while adding concentrated HCl 3 during this time, the mixture cooled, EtOH removed in vacuo, the precipitate dissolved in the necessary amount of H2O, the solution extracted with Et2O (from the extract I 110-15 was recovered), made alkaline with K2CO3 and a little NaOH solution, the base taken up in Et2O, the Et2O solution washed with H2O, dried, evaporated, and the residue 152 parts distilled gave 2-CH2NMe2 derivative of I, b8 105-10° (HCl salt, m. 138-9°; methiodide, m. 182-4°). Similarly were prepared the following derivs. of I (2-substituent, b.p./mm., m.p. of HCl salt, m.p. of methiodide given): morpholinomethyl, 120-6°/0.2, 150°, 171-4°; piperidinomethyl, 112-15°/0.2, 155-6°, 126-8°; hexamethyleniminomethyl, 121-4°/0.2, 146-7°,

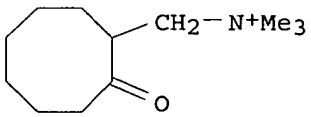
154-7°; Et2NCH2, 78-84°/0.2, 106-7°, -;
pyrrolidinomethyl, 106-11°/0.2, 142.5-4.0°, 97-9.5°.

IT **28118-62-9**, Cyclooctanone, 2-(dimethylaminomethyl)-
61977-58-0, Ammonium, trimethyl(2-oxocyclooctylmethyl)-, iodide
100049-46-5, Cyclooctanone, 2-(dimethylaminomethyl)-,
hydrochloride **100539-21-7**, Cyclooctanone, 2-(diethylaminomethyl)-
, hydrochloride **100539-22-8**, Cyclooctanone, 2-
(diethylaminomethyl)- **101172-06-9**, Cyclooctanone,
2-morpholinomethyl-, hydrochloride **101172-07-0**, Cyclooctanone,
2-morpholinomethyl-
(preparation of)

RN 28118-62-9 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]- (6CI, 8CI, 9CI) (CA INDEX NAME)

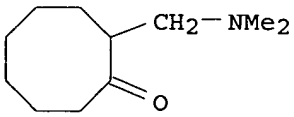


RN 61977-58-0 CAPLUS
CN Cyclooctanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



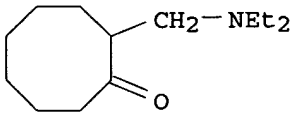
● I^-

RN 100049-46-5 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]-, hydrochloride (6CI, 9CI) (CA INDEX NAME)



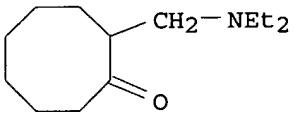
● HCl

RN 100539-21-7 CAPLUS
CN Cyclooctanone, 2-(diethylaminomethyl)-, hydrochloride (6CI) (CA INDEX NAME)

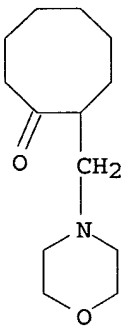


● HCl

RN 100539-22-8 CAPLUS
CN Cyclooctanone, 2-[(diethylamino)methyl]- (6CI, 9CI) (CA INDEX NAME)

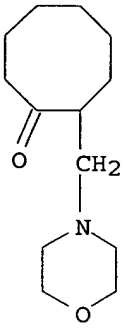


RN 101172-06-9 CAPLUS
CN Cyclooctanone, 2-morpholinomethyl-, hydrochloride (6CI) (CA INDEX NAME)



● HCl

RN 101172-07-0 CAPLUS
CN Cyclooctanone, 2-morpholinomethyl- (6CI) (CA INDEX NAME)



L9 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1959:40054 CAPLUS
DOCUMENT NUMBER: 53:40054
ORIGINAL REFERENCE NO.: 53:7217e-i,7218a-b
TITLE: Diphenylmethane and 1-azadibenzo [2,3;5,6] cycloheptadiene derivatives
INVENTOR(S): Martin, Henry; Habicht, Ernst
PATENT ASSIGNEE(S): Cilag Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

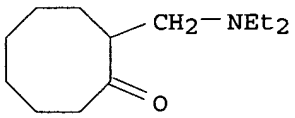
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2861987		19581125	US 1956-630777	19561227
DE 1084267			DE	

ED Entered STN: 22 Apr 2001
AB The title compds. (I and II, resp.), useful as antihistamine agents and as analgesics, were prepared o-MeNHC6H4CH2Ph (III) (15 g.) in 100 cc. absolute PhMe mixed with 3.9 g. NaNH2 in 50 cc. PhMe, 12.2 g. Me2NCH2CH2CH2Cl (IV) in 500 cc. absolute PhMe added, the mixture heated and stirred several hrs.
at 110°, cooled, extracted with 50 cc. 2N aqueous Na2CO3, the PhMe layer dried, evaporated to dryness in vacuo, the residue mixed with 50 cc. 2N AcOH, the precipitate filtered off, washed with 50 cc. 2N AcOH and H2O, the filtrate made alkaline with 100 cc. saturated K2CO3, the alkaline solution extracted with AcOH, the
acid solution made alkaline with 100 cc. saturated aqueous K2CO3, the separated oil dried,
and distilled gave 5-10 g. o-[N-methyl-N-(3-dimethylaminopropyl)amino]diphenylmethane, b0.09 140-3° (HCl salt, m. 136-7°; methosulfate, m. 97-8°). Similarly were prepared o-[N-methyl-N-(2-dimethylaminoethyl)amino]diphenylmethane, b0.07 130-2° (HCl salt, m. 183-4°; methosulfate, m. 128-9°); o-[N-ethyl-N-(2-pyrrolidinoethyl)amino]diphenylmethane, b0.015 136-7°; o-[N-propyl-N-(2-piperidinoethyl)amino]diphenylmethane, b0.03 145-7°; o-[N-(1-methyl-3-pyrrolidylmethyl)-N-methylamino]diphenylmethane, b0.02 146° (HCl salt, m. 133-5°; methosulfate, m. 80-1°). ClCH2COCl (V) added with stirring and cooling to o-H2NC6H4CH2Ph and Et3N in C6H6 gave o-ClCH2CONHC6H4CH2Ph (VI), m. 113-14°. VI in C6H6 heated several hrs. with Et2NH gave 62% o-Et2NCH2CONHC6H4CH2Ph (VII), m. 67-8° (HCl salt, m.

204-6°); VII and its homologs have a strong anesthetic effect. VII in C6H6 added to 7.6 g. LiAlH4 in tetrahydrofuran (VIII)-C6H6 gave o-(2-diethylaminoethylamino)diphenylmethane (IX), b0.05 151-3° (HCl salt, m. 139-40°). IX treated with CH2O and HCO2H gave the N-Me derivative (X), b0.02 133-6° (HCl salt, m. 122-4°; methosulfate, m. 65°). X was also prepared by treating III with V to form o-(ClCH2CONMe)C6H4CH2Ph (XI), m. 53-4°, treating XI with Et2NH to form o-(Et2NCH2CONMe)C6H4CH2Ph, b0.02 148-50°, and reducing (LiAlH4) the latter. 1-Azadibenzo[2,3;5,6]cycloheptadiene (XII) (100 g.), 31 g. NaNH2, and 122 g. IV in xylene boiled several hrs. gave 49 g. 1-Me2N(CH2)3 derivative, b0.1 141-3° (HCl salt, m. 176-8°). Similarly were prepared the following 1-substituted derivs. of XII (1-substituent and b.p./mm. given): 3-pyrrolidinopropyl, 151-3°/0.01; 3-piperidinopropyl, 165-6°/0.02; 2-pyrrolidinopropyl, 152-3°/0.01; Et2N(CH2)3, 161-2°/0.015; 2-(1-methylpiperazinyl)ethyl, 160-3°/0.01; 2-morpholinoethyl, 161-4°/0.03; Et2NCH2CH2 (XIII), 140-5°/0.01. XII and V treated in VIII-dioxane (XIV) gave 78% 1-ClCH2CO derivative (XV), m. 137-8° XV and Et2NH in XIV boiled 2 hrs. gave 74% 1-Et2NCH2CO derivative of XII, b0.03 180-1°, which treated with LiAlH4 in VIII gave XIII, b0.01 140-5°.

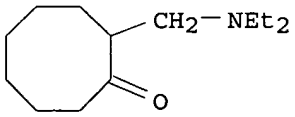
IT **100539-21-7**, Cyclooctanone, 2-(diethylaminomethyl)-, hydrochloride
100539-22-8, Cyclooctanone, 2-(diethylaminomethyl)-
109474-04-6, 4-Methyl-4-(2-oxocyclooctylmethyl)morpholinium iodide
(preparation of)

RN 100539-21-7 CAPLUS
CN Cyclooctanone, 2-(diethylaminomethyl)-, hydrochloride (6CI) (CA INDEX NAME)

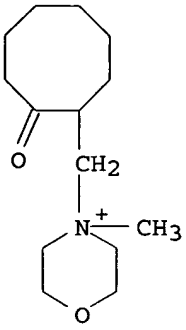


● HCl

RN 100539-22-8 CAPLUS
CN Cyclooctanone, 2-[(diethylamino)methyl]- (6CI, 9CI) (CA INDEX NAME)



RN 109474-04-6 CAPLUS
CN 4-Methyl-4-(2-oxocyclooctylmethyl)morpholinium iodide (6CI) (CA INDEX NAME)

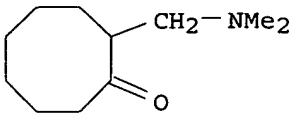


L9 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1958:113300 CAPLUS
DOCUMENT NUMBER: 52:113300
ORIGINAL REFERENCE NO.: 52:19983i,19984a-b
TITLE: Alicyclic amino ketones
PATENT ASSIGNEE(S): Badische Anilin- & Soda-Fabrik Akt.-Ges.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

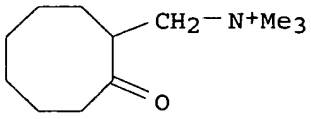
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 792190		19580319	GB	

ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB The title compds., having analgesic properties, were prepared by treating cyclooctanone (I) with CH2O and secondary amines. Thus, I 252, Me2NH.HCl 81.5, CH2O 39, and EtOH 320 was refluxed 105 min. while concentrated HCl 3 parts was added. The EtOH was removed, the HCl salt dissolved in H2O, and the excess I (110-15 parts) removed by Et2O extraction The aqueous phase was neutralized, extracted with Et2O, the extract washed and dried, and the Et2O evaporated to give 2-(dimethylaminomethyl)cyclooctan-1-one 152 parts, b8 105-10°; HCl salt, m. 138-9°; MeI salt, m. 182-4°.
Similarly were prepared the following 2-(R-methyl)cyclooctanones (R, b.p./0.2 mm., m.p. of HCl salt, m.p. of MeI salt, and yield in x parts from y parts of I given): morpholino, 120-6°, 150°, 171-4°, 178 from 252; piperidino, 112-15°, 155°, 126-8°. 70 from 126; CH2.(CH2)5.N, 121-4°, 146-7°, 154-7°, 108 from 252; Et2N, 78-84°, 106-7°, -, 80 from 252; CH2.(CH2)3.N, 106-11°, 142.5-4.0°, 97.0-9.5°, 64 from 126.
IT **28118-62-9**, Cyclooctanone, 2-(dimethylaminomethyl)-
61977-58-0, Ammonium, trimethyl(2-oxocyclooctylmethyl)-, iodide
100049-46-5, Cyclooctanone, 2-(dimethylaminomethyl)-, hydrochloride **100539-21-7**, Cyclooctanone, 2-(diethylaminomethyl)-, hydrochloride **101172-06-9**, Cyclooctanone, 2-morpholinomethyl-, hydrochloride **101172-07-0**, Cyclooctanone, 2-morpholinomethyl-
109474-04-6, 4-Methyl-4-(2-oxocyclooctylmethyl)morpholinium iodide

(preparation of)
RN 28118-62-9 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]- (6CI, 8CI, 9CI) (CA INDEX NAME)

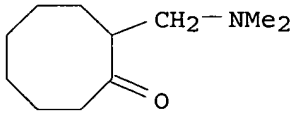


RN 61977-58-0 CAPLUS
CN Cyclooctanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



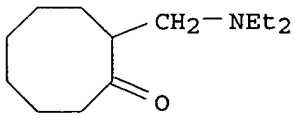
● I^-

RN 100049-46-5 CAPLUS
CN Cyclooctanone, 2-[(dimethylamino)methyl]-, hydrochloride (6CI, 9CI) (CA INDEX NAME)



● HCl

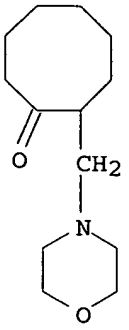
RN 100539-21-7 CAPLUS
CN Cyclooctanone, 2-(diethylaminomethyl)-, hydrochloride (6CI) (CA INDEX NAME)



● HCl

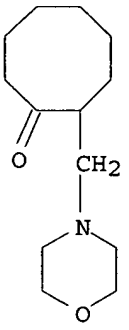
RN 101172-06-9 CAPLUS

CN Cyclooctanone, 2-morpholinomethyl-, hydrochloride (6CI) (CA INDEX NAME)

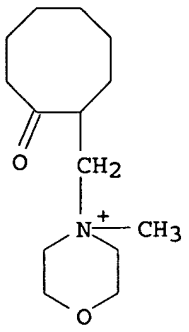


● HCl

RN 101172-07-0 CAPLUS
CN Cyclooctanone, 2-morpholinomethyl- (6CI) (CA INDEX NAME)



RN 109474-04-6 CAPLUS
CN 4-Methyl-4-(2-oxocyclooctylmethyl)morpholinium iodide (6CI) (CA INDEX NAME)



● I^-

L9 ANSWER 26 OF 26 USPATFULL on STN

ACCESSION NUMBER:	2005:234237 USPATFULL
TITLE:	Methods for selectively inhibiting janus tyrosine kinase 3 (JAK3)
INVENTOR(S):	Kirken, Robert A., Conroe, TX, UNITED STATES Kahan, Barry D., Houston, TX, UNITED STATES Stepkowski, Stanislaw M., Pearland, TX, UNITED STATES Priebe, Waldemar, Houston, TX, UNITED STATES Fokt, Izabela, Spring, TX, UNITED STATES Kosinski, Szymon, Menomonee Falls, WI, UNITED STATES
PATENT ASSIGNEE(S):	Board of Regents,The University of Texas System, Austin, TX, UNITED STATES (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2005203177	A1	20050915	
APPLICATION INFO.:	US 2003-731769	A1	20031209	(10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-431851P	20021209 (60)

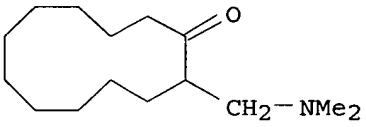
DOCUMENT TYPE:	Utility
FILE SEGMENT:	APPLICATION
LEGAL REPRESENTATIVE:	CONLEY ROSE, P.C., P. O. BOX 3267, HOUSTON, TX, 77253-3267, US
NUMBER OF CLAIMS:	33
EXEMPLARY CLAIM:	1
NUMBER OF DRAWINGS:	18 Drawing Page(s)
LINE COUNT:	1898

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Methods are disclosed for inhibiting or disrupting Janus tyrosine kinase 3 (Jak3) dependent function in cells of lymphoid or myeloid origin, especially for blocking proliferation and function of lymphocytes (e.g., T-cells, B-cells). A Mannich base compound, or a derivative or modified compound, is employed which is capable of selectively inhibiting Jak3 while affecting other protein tyrosine kinase activities to a lesser extent or not at all, to provide beneficial effects such as mitigation of transplant rejection and alleviation of allergic responses with fewer side effects than with conventional immunosuppressive agents.

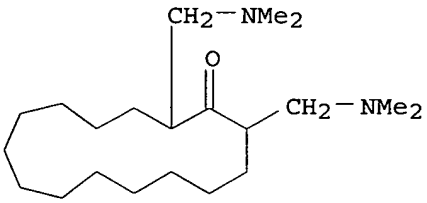
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **14519-21-2 150661-92-0 173543-81-2**
708984-86-5 708984-86-5D, salts **708984-87-6**
708984-87-6D, salts **708984-88-7 708984-89-8**
708984-90-1 708984-91-2 708984-92-3
708984-93-4 708984-94-5 708984-95-6
708984-98-9 708984-99-0 708985-00-6
708985-01-7 708985-02-8 708985-03-9
708985-04-0 708985-05-1 708985-06-2
708985-07-3
(selectively inhibiting Janus tyrosine kinase 3 with Mannich base compds. for mitigation of transplant rejection and allergies)

RN 14519-21-2 USPATFULL
CN Cyclododecanone, 2-[(dimethylamino)methyl]-, hydrochloride (8CI, 9CI) (CA INDEX NAME)



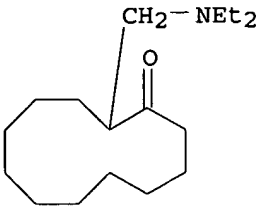
● HCl

RN 150661-92-0 USPATFULL
CN Cyclopentadecanone, 2,15-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



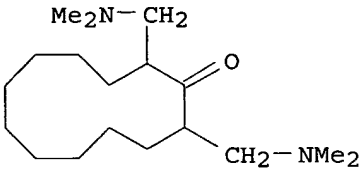
●2 HCl

RN 173543-81-2 USPATFULL
CN Cyclododecanone, 2-[(diethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)

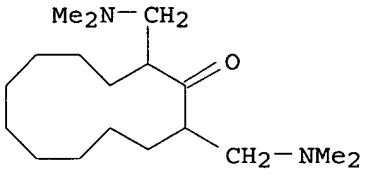


● HCl

RN 708984-86-5 USPATFULL
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]- (9CI) (CA INDEX NAME)

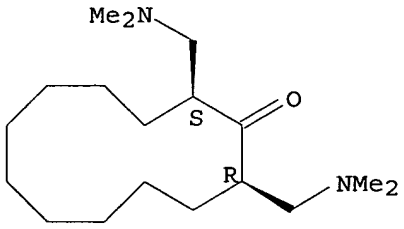


RN 708984-86-5 USPATFULL
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]- (9CI) (CA INDEX NAME)



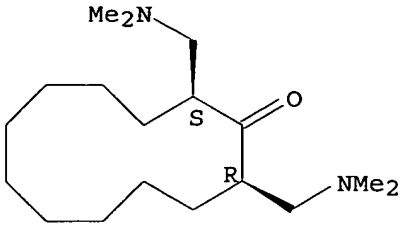
RN 708984-87-6 USPATFULL
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, (2R,12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

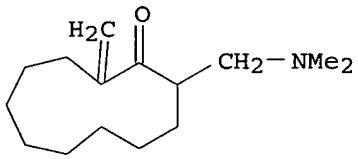


RN 708984-87-6 USPATFULL
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, (2R,12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

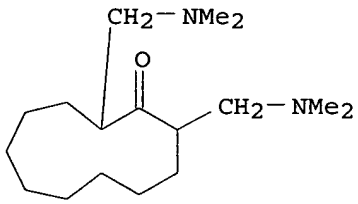


RN 708984-88-7 USPATFULL
CN Cycloundecanone, 2-[(dimethylamino)methyl]-11-methylene-, hydrochloride (9CI) (CA INDEX NAME)



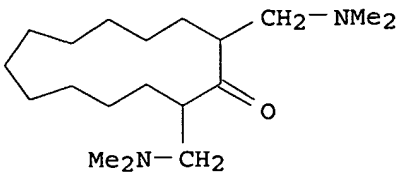
● HCl

RN 708984-89-8 USPATFULL
CN Cycloundecanone, 2,11-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

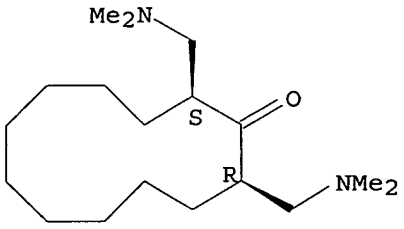
RN 708984-90-1 USPATFULL
CN Cyclotridecanone, 2,13-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

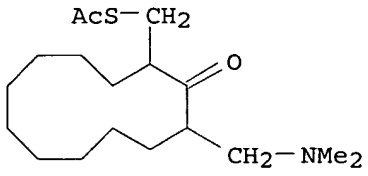
RN 708984-91-2 USPATFULL
CN Cyclododecanone, 2,12-bis[(dimethylamino)methyl]-, dihydrochloride, (2R,12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



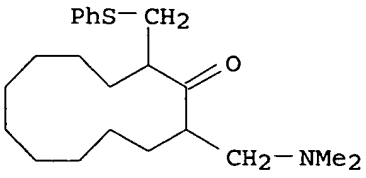
●2 HCl

RN 708984-92-3 USPATFULL
CN Ethanethioic acid, S-[[3-[(dimethylamino)methyl]-2-oxocyclododecyl]methyl] ester, hydrochloride (9CI) (CA INDEX NAME)



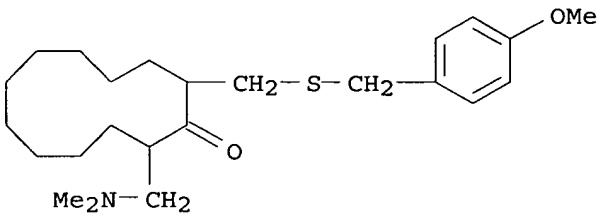
● HCl

RN 708984-93-4 USPATFULL
CN Cyclododecanone, 2-[(dimethylamino)methyl]-12-[(phenylthio)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



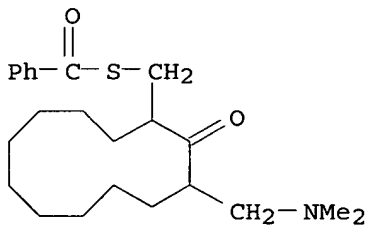
● HCl

RN 708984-94-5 USPATFULL
CN Cyclododecanone, 2-[(dimethylamino)methyl]-12-[[[(4-methoxyphenyl)methyl]thio]methyl]-, hydrochloride (9CI) (CA INDEX NAME)



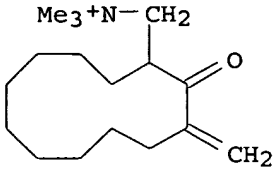
● HCl

RN 708984-95-6 USPATFULL
CN Benzenecarbothioic acid, S-[[3-[(dimethylamino)methyl]-2-oxocyclododecyl]methyl] ester, hydrochloride (9CI) (CA INDEX NAME)



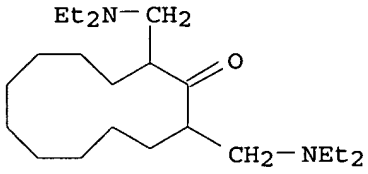
● HCl

RN 708984-98-9 USPATFULL
CN Cyclododecanemethanaminium, N,N,N-trimethyl-3-methylene-2-oxo-, iodide (9CI) (CA INDEX NAME)



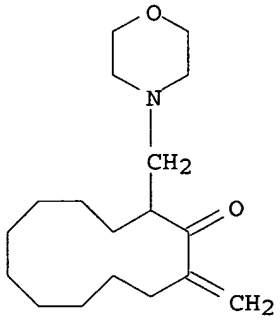
● I-

RN 708984-99-0 USPATFULL
CN Cyclododecanone, 2,12-bis[(diethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



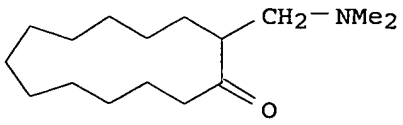
●2 HCl

RN 708985-00-6 USPATFULL
CN Cyclododecanone, 2-methylene-12-(4-morpholinylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)



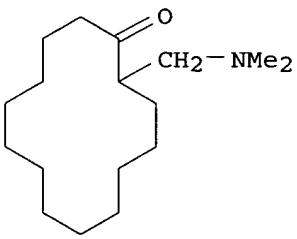
● HCl

RN 708985-01-7 USPATFULL
CN Cyclotridecanone, 2-[(dimethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



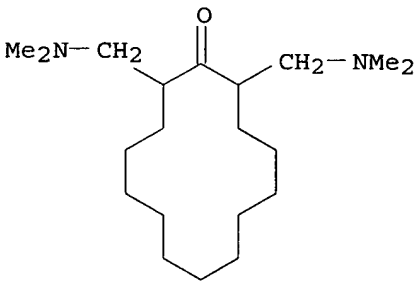
● HCl

RN 708985-02-8 USPATFULL
CN Cyclotetradecanone, 2-[(dimethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



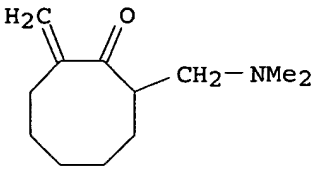
● HCl

RN 708985-03-9 USPATFULL
CN Cyclotetradecanone, 2,14-bis[(dimethylamino)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



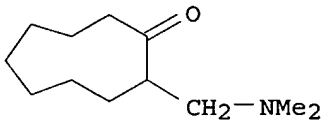
●2 HCl

RN 708985-04-0 USPATFULL
CN Cyclooctanone, 2-[(dimethylamino)methyl]-8-methylene-, hydrochloride (9CI) (CA INDEX NAME)



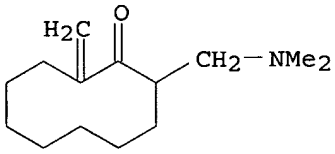
● HCl

RN 708985-05-1 USPATFULL
CN Cyclononanone, 2-[(dimethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



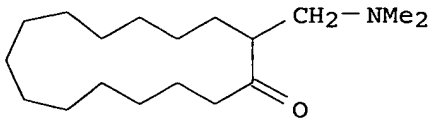
● HCl

RN 708985-06-2 USPATFULL
CN Cyclodecanone, 2-[(dimethylamino)methyl]-10-methylene-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 708985-07-3 USPATFULL
CN Cyclopentadecanone, 2-[(dimethylamino)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

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This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

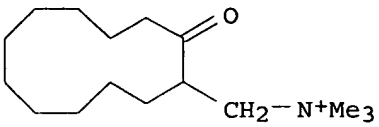
L10 8 L5

=> d iall hitstr l10 1-8; fil hom

L10 ANSWER 1 OF 8 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA58:10104b CAOLD
TITLE: cyclooctatetraene
AUTHOR NAME: Pirzer, Hans; Stadler, R.; Becke, F.
PATENT ASSIGNEE: Badische Anilin- & Soda-Fabrik A.-G.
DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
PI DE 1138763		

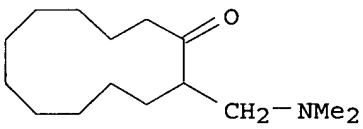
INDEX TERM: 16215-59-1 **16277-21-7** 16277-22-8 94980-98-0
IT **16277-21-7**
RN 16277-21-7 CAOLD
CN Cyclododecanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



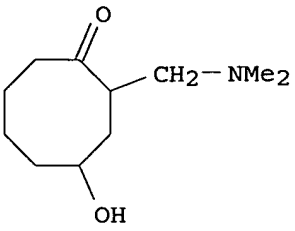
L10 ANSWER 2 OF 8 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA58:10104a CAOLD
TITLE: 1-ketocyclododecyl-2-AcOH as a choleretic
PATENT ASSIGNEE: Chimie et Atomistique
DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
FR M100		

INDEX TERM: 16215-59-1 **16215-60-4** 94980-98-0
IT **16215-60-4**
RN 16215-60-4 CAOLD
CN Cyclododecanone, 2-[(dimethylamino)methyl]- (7CI, 8CI, 9CI) (CA INDEX NAME)

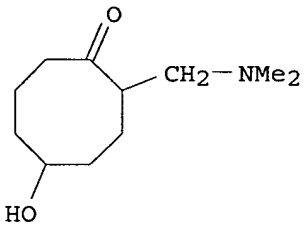


L10 ANSWER 3 OF 8 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA56:9992d CAOLD
TITLE: products of the catalytic oxidation of cyclooctane
AUTHOR NAME: Moell, Hans; Urbanek, F.
INDEX TERM: 284-20-8 286-62-4 696-71-9 4277-32-1 5388-47-6
6925-14-0 10515-92-1 55343-44-7 55794-44-0 61755-97-3
90191-65-4 90204-13-0 90204-14-1 90204-83-4 90204-84-5
90226-59-8 90226-60-1 90608-88-1 91005-62-8 91005-63-9
91056-73-4 **91370-52-4** **91370-53-5**
92373-80-3 92373-81-4 92971-32-9 97468-82-1 97468-83-2
IT **91370-52-4** **91370-53-5**
RN 91370-52-4 CAOLD
CN Cyclooctanone, 2-[(dimethylamino)methyl]-4-hydrOxy-, hydrochloride (7CI) (CA INDEX NAME)



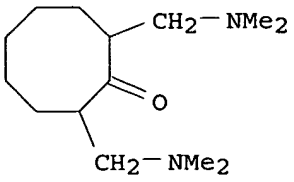
● HCl

RN 91370-53-5 CAOLD
CN Cyclooctanone, 2-[(dimethylamino)methyl]-5-hydroxy-, hydrochloride (7CI) (CA INDEX NAME)



● HCl

L10 ANSWER 4 OF 8 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA54:5507g CAOLD
TITLE: disubstitution of cycloalkanones in the Mannich reaction
AUTHOR NAME: Blicke, Frederick F.; McCarty, F. J.
INDEX TERM: **6333-26-2** 6333-27-3 6333-28-4 6333-29-5
6333-30-8 6940-21-2 7477-26-1 7507-57-5 13290-49-8
15409-60-6 25928-05-6 37408-85-8 42036-65-7 98552-17-1
98998-28-8 100387-55-1 101591-56-4 101780-21-6 102176-49-8
102596-84-9 102897-85-8 103157-26-2 103267-78-3 103277-15-2
103330-06-9 103401-85-0 103755-77-7 104035-85-0 105912-13-8
105974-91-2 107059-65-4 107525-09-7 107924-12-9 108989-23-7
108992-37-6 110437-08-6 113011-25-9 113861-29-3 114159-42-1
114159-70-5 119075-02-4 122218-51-3
IT **6333-26-2**
RN 6333-26-2 CAOLD
CN Cyclooctanone, 2,8-bis[(dimethylamino)methyl]-, dihydrochloride (6CI, 8CI, 9CI) (CA INDEX NAME)

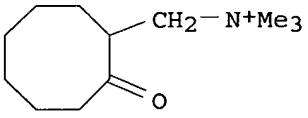


● 2 HCl

L10 ANSWER 5 OF 8 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA53:21721a CAOLD
TITLE: 1-oxocyclooctyl-2-acetic acid
AUTHOR NAME: Schlichting, Otto; Scheuerer, G.
PATENT ASSIGNEE: Badische Anilin- & Soda-Fabrik Akt.-Ges.
DOCUMENT TYPE: Patent

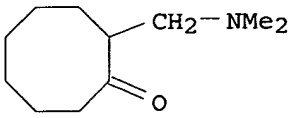
PATENT NO.	KIND	DATE
US 2882292		1959

INDEX TERM: 19144-09-3 **61977-58-0 100049-46-5** 100051-98-7 100131-66-6 101275-22-3 **108903-90-8** 131239-93-5
IT **61977-58-0 100049-46-5 108903-90-8**
RN 61977-58-0 CAOLD
CN Cyclooctanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



● I^-

RN 100049-46-5 CAOLD
CN Cyclooctanone, 2-[(dimethylamino)methyl]-, hydrochloride (6CI, 9CI) (CA INDEX NAME)

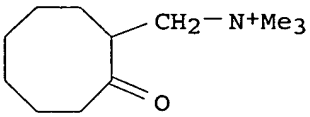


● HCl

RN 108903-90-8 CAOLD
CN Trimethyl(2-oxocyclooctylmethyl)ammonium methyl sulfate (6CI) (CA INDEX NAME)

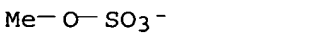
CM 1

CRN 108903-89-5
CMF C12 H24 N O



CM 2

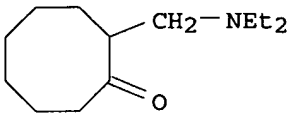
CRN 21228-90-0
CMF C H3 O4 S



L10 ANSWER 6 OF 8 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA53:7217e CAOLD
TITLE: 2-disubstituted(aminomethyl) cyclooctanones
PATENT ASSIGNEE: Badische Anilin- & Soda-Fabrik Akt.-Ges.
DOCUMENT TYPE: Patent
TITLE: diphenyl methane and 1-azadibenzo[2,3:5,6]-cycloheptadiene derivs.
PATENT ASSIGNEE: Cilag-Chemie Ltd.
DOCUMENT TYPE: Patent
TITLE: diphenylmethane and 1-azadibenzo[2,3:5,6]cycloheptadiene derivs.
AUTHOR NAME: Martin, Henry; Habicht, E.
DOCUMENT TYPE: Patent

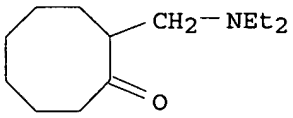
	PATENT NO.	KIND	DATE
PI	US 2861987		1958
	DE 1084267		

INDEX TERM: 73-07-4 966-90-5 3046-01-3 21535-43-3 64125-21-9
93010-71-0 **100539-21-7 100539-22-8**
100877-62-1 101171-80-6 101171-81-7 **101172-06-9**
101172-07-0 101737-52-4 102166-72-3 102166-80-3
102166-84-7 102453-37-2 102552-40-9 102753-46-8 109407-18-3
109451-98-1 **109474-04-6** 109499-47-0 109499-48-1
109701-19-1 109935-24-2 110249-32-6 110876-70-5 110877-37-7
111356-98-0 112247-76-4 112272-25-0 112554-00-4 112574-94-4
113651-88-0 113951-40-9 113951-41-0 114004-75-0 114889-22-4
114911-05-6 116130-62-2 122803-48-9 131239-93-5
IT **100539-21-7 100539-22-8 101172-06-9**
101172-07-0 109474-04-6
RN 100539-21-7 CAOLD
CN Cyclooctanone, 2-(diethylaminomethyl)-, hydrochloride (6CI) (CA INDEX NAME)

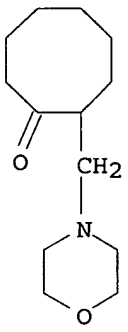


● HCl

RN 100539-22-8 CAOLD
CN Cyclooctanone, 2-[(diethylamino)methyl]- (6CI, 9CI) (CA INDEX NAME)

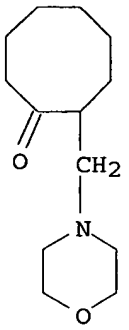


RN 101172-06-9 CAOLD
CN Cyclooctanone, 2-morpholinomethyl-, hydrochloride (6CI) (CA INDEX NAME)

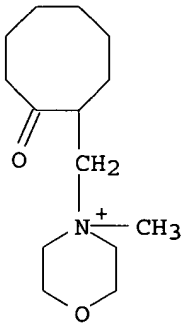


● HCl

RN 101172-07-0 CAOLD
CN Cyclooctanone, 2-morpholinomethyl- (6CI) (CA INDEX NAME)



RN 109474-04-6 CAOLD
CN 4-Methyl-4-(2-oxocyclooctylmethyl)morpholinium iodide (6CI) (CA INDEX NAME)

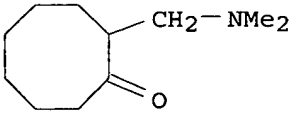


● I^-

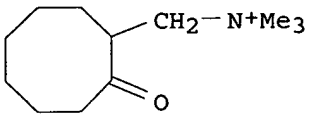
L10 ANSWER 7 OF 8 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA53:7217c CAOLD
TITLE: 2-(disubstituted aminomethyl) cyclooctanones
AUTHOR NAME: Schlichting, Otto; Scheuerer, G.; Westphal, F.; Amann, A.
DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
US 2861993		1958

INDEX TERM: **28118-62-9 61977-58-0 100049-46-5** 109185-96-8 115486-15-2 115486-16-3
IT **28118-62-9 61977-58-0 100049-46-5**
RN 28118-62-9 CAOLD
CN Cyclooctanone, 2-[(dimethylamino)methyl]- (6CI, 8CI, 9CI) (CA INDEX NAME)

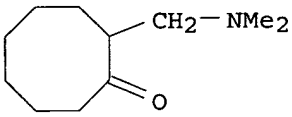


RN 61977-58-0 CAOLD
CN Cyclooctanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



● I^-

RN 100049-46-5 CAOLD
CN Cyclooctanone, 2-[(dimethylamino)methyl]-, hydrochloride (6CI, 9CI) (CA INDEX NAME)

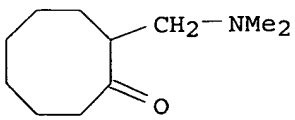


● HCl

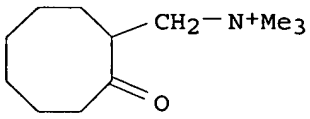
L10 ANSWER 8 OF 8 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA52:19983i CAOLD
TITLE: amino ketones (alicyclic)
PATENT ASSIGNEE: Badische Anilin- & Soda-Fabrik Akt.-Ges.
DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
GB 792190		

INDEX TERM: 3046-01-3 **28118-62-9 61977-58-0**
100049-46-5 100539-21-7
100539-22-8 100877-62-1 101171-80-6 101171-81-7
101172-06-9 101172-07-0 109407-18-3
109451-98-1 **109474-04-6** 109499-47-0 109499-48-1
131239-93-5
IT **28118-62-9 61977-58-0 100049-46-5**
100539-21-7 100539-22-8 101172-06-9
101172-07-0 109474-04-6
RN 28118-62-9 CAOLD
CN Cyclooctanone, 2-[(dimethylamino)methyl]- (6CI, 8CI, 9CI) (CA INDEX NAME)

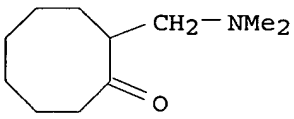


RN 61977-58-0 CAOLD
CN Cyclooctanemethanaminium, N,N,N-trimethyl-2-oxo-, iodide (9CI) (CA INDEX NAME)



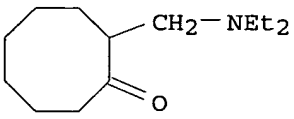
● I^-

RN 100049-46-5 CAOLD
CN Cyclooctanone, 2-[(dimethylamino)methyl]-, hydrochloride (6CI, 9CI) (CA INDEX NAME)



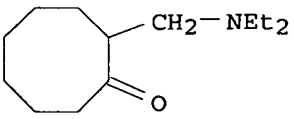
● HCl

RN 100539-21-7 CAOLD
CN Cyclooctanone, 2-(diethylaminomethyl)-, hydrochloride (6CI) (CA INDEX NAME)

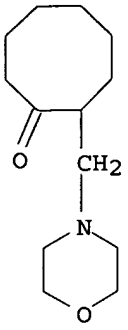


● HCl

RN 100539-22-8 CAOLD
CN Cyclooctanone, 2-[(diethylamino)methyl]- (6CI, 9CI) (CA INDEX NAME)

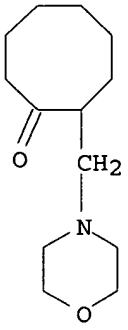


RN 101172-06-9 CAOLD
CN Cyclooctanone, 2-morpholinomethyl-, hydrochloride (6CI) (CA INDEX NAME)

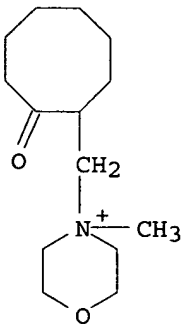


● HCl

RN 101172-07-0 CAOLD
CN Cyclooctanone, 2-morpholinomethyl- (6CI) (CA INDEX NAME)



RN 109474-04-6 CAOLD
CN 4-Methyl-4-(2-oxocyclooctylmethyl)morpholinium iodide (6CI) (CA INDEX NAME)



● I^-

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